

LPS effect- metabolomics pilot study on liver samples (identified and annotated metabolites)

CTL T0h vs CTL T12h

<i>Peak id</i>	<i>Metabolite</i>	<i>log fc</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T0h</i>	<i>Peak intensity CTL T12h</i>	<i>Identification</i>
1	Betaine	-1.04	0.0000	0.0000	2705088320	1320054272	identified+fragment
12	L-isoleucyl-L-proline	-1.76	0.0000	0.0000	2848519	840496	annotated
13	Prolyl-Valine	-1.95	0.0000	0.0000	1047546	271849	annotated
14	Pterolactam	-1.06	0.0000	0.0000	682330064	328330992	annotated+fragment
15	Dulxanthone F	-0.83	0.0000	0.0000	9515978	5341230	annotated+fragment
16	Hydroxyprolyl-Valine	-1.69	0.0000	0.0000	1583226	489352	annotated
23	Neurine	-1.48	0.0000	0.0000	359767004	128920014	annotated
31	Hypoxanthine	-2.35	0.0000	0.0000	369858112	72556805	identified+fragment
116	L-Valine	-1.81	0.0000	0.0000	118959670	33855504	identified+fragment
33	Pyridine N-oxide glucuronide	-4.37	0.0000	0.0000	3637254	175750	annotated
35	5-Hydroxytryptophan	-1.98	0.0000	0.0000	541184	137047	annotated
51	Homocarnosine	-1.60	0.0000	0.0000	6945894	2292955	annotated+fragment
59	L-Alloisoleucine	-1.69	0.0000	0.0000	201673344	62714576	annotated+fragment
137	L-Methionine	-1.88	0.0000	0.0000	88358132	24088644	identified+fragment
61	Sakacin P	-1.42	0.0000	0.0000	1450810	541157	annotated
66	Guanidinoacetate	-2.56	0.0000	0.0000	151638978	25657283	annotated+fragment
70	Polixetonium chloride	-3.04	0.0000	0.0000	718029	87123	annotated
74	Gentianose	-3.04	0.0000	0.0000	269253	32641	annotated
76	6-(alpha-D-Glucosaminy1)-1D-myo-inositol	-3.06	0.0000	0.0000	237313	28495	annotated
79	cis-N-Methyl-(S)-7,8,13,14-tetrahydroprotoberberine	-2.61	0.0000	0.0000	216235	35352	annotated
83	beta-D-Galactopyranosyl-(1->4)-2-amino-2-deoxy-beta-D-glucopyranosyl-(1->6)-D-mannose	-2.82	0.0000	0.0000	138242	19527	annotated
85	Dictyoquinazol B	-4.66	0.0000	0.0000	105806	4176	annotated

91	2S-amino-butanoic acid	-1.20	0.0000	0.0000	127190702	55504337	annotated+fragment
94	Methyl N-methylantranilate	-1.51	0.0000	0.0000	139686506	48989941	annotated+fragment
95	L-gamma-glutamyl-L-leucine	-2.36	0.0000	0.0000	2381021	463935	annotated
146	beta-Alanine	-1.55	0.0000	0.0000	109481032	37497190	identified
149	L-Arginine	-1.34	0.0000	0.0000	90412425	35638168	identified+fragment
168	Nicotinamide	-1.78	0.0000	0.0000	69032133	20070509	identified+fragment
119	Sesamolin	-2.61	0.0000	0.0000	2488442	408032	annotated
170	L-homoserine	-1.25	0.0000	0.0000	74107600	31158635	identified+fragment
209	L-Tyrosine	-1.81	0.0000	0.0000	55242248	15791040	identified+fragment
266	L-Serine	-1.34	0.0000	0.0000	27032162	10665263	identified+fragment
411	L-Ornithine	-2.48	0.0000	0.0000	8423028	1508908	identified+fragment
164	PC(18:1(9Z)/18:1(9Z))	-0.78	0.0000	0.0000	92996812	54042310	annotated
448	Creatinine	-1.03	0.0000	0.0000	10594521	5180474	identified+fragment
2804	pyrophosphate	-5.25	0.0000	0.0000	9390607	246005	identified
171	(5-L-Glutamyl)-L-glutamine	-1.85	0.0000	0.0000	2630942	732089	annotated
173	Alanyl-Aspartate	-1.68	0.0000	0.0000	1104428	343663	annotated
175	Aspartyl-Proline	-2.02	0.0000	0.0000	764180	187787	annotated
176	L-Tyrosine	-1.61	0.0000	0.0000	406807	133443	annotated
187	Pantothenic acid	-2.43	0.0000	0.0000	55220356	10256678	annotated+fragment
188	S-Acetyldihydrolipoamide	-1.27	0.0000	0.0000	54330600	22600569	annotated
207	NG,NG-Dimethyl-L-arginine	-2.65	0.0000	0.0000	38060983	6069091	annotated
2830	L-Aspartate	-1.27	0.0000	0.0000	73662101	30596196	identified
214	Hydroxypropyl-Serine	-2.17	0.0000	0.0000	1438368	319893	annotated
216	Gamma-Glutamyltyrosine	-1.25	0.0000	0.0000	536367	225294	annotated
2838	CMP	-2.28	0.0000	0.0000	1093147	225561	identified+fragment
252	PC(18:0/0:0)	-1.48	0.0000	0.0000	46189582	16548640	annotated+fragment
2993	L-isoleucine	-2.09	0.0000	0.0000	24940411	5873168	identified
3066	Orotate	-2.12	0.0000	0.0000	1025379	235142	identified
278	PC(18:2(9Z,12Z)/0:0)	-1.57	0.0000	0.0000	33781739	11410159	annotated
281	Ergothioneine	-1.24	0.0000	0.0000	29430552	12457578	annotated

282	Tetrahydropentoxylane	-1.06	0.0000	0.0000	2316037	1113319	annotated
291	PC(15:0/0:0)	-1.81	0.0000	0.0000	29771136	8484744	annotated
296	Allopurinol riboside	-1.36	0.0000	0.0000	28602452	11166082	annotated+fragment
316	Indoleacrylic acid	-1.96	0.0000	0.0000	18805457	4839188	annotated
317	N2-Acetyl-L-aminoadipate	-2.17	0.0000	0.0000	8229142	1823097	annotated
318	N-Acetyl-beta-D-galactosamine	-2.22	0.0000	0.0000	3758856	804667	annotated+fragment
320	Gamma-glutamyl-Proline	-1.76	0.0000	0.0000	1549246	458306	annotated
326	Piperidine	-1.33	0.0000	0.0000	19576103	7762063	annotated+fragment
337	1-(beta-D-Ribofuranosyl)-1,4-dihyronicotinamide	-2.82	0.0000	0.0000	11325127	1609322	annotated
385	LysoPC(18:1(11Z))	-2.65	0.0000	0.0000	1459846	232796	annotated
409	1,4-Dideoxy-1,4-imino-D-ribitol	-1.44	0.0000	0.0000	9488861	3487772	annotated
3422	L-Tryptophan	-1.54	0.0000	0.0000	3125259	1071355	identified
416	(S)-Codamine	-3.76	0.0000	0.0000	83982	6209	annotated
422	(5-L-Glutamyl)-L-glutamate	-3.52	0.0000	0.0000	7301280	635704	annotated+fragment
423	Cysteineglutathione disulfide	-2.44	0.0000	0.0000	909965	167310	annotated
438	(3S)-3-Hydroxy-L-enduracididine	-2.88	0.0000	0.0000	9612745	1307892	annotated
474	2,3-Dihydro-2,3-dihydroxy-4-(4-methoxyphenyl)-1H-phenalen-1-one	-1.75	0.0000	0.0000	125147	37166	annotated
605	PS(18:0/20:4(8Z,11Z,14Z,17Z))	1.03	0.0000	0.0000	3925743	8038163	annotated
612	PG(P-16:0/20:3(8Z,11Z,14Z))	-1.98	0.0000	0.0000	219480	55502	annotated
640	2-Aminoheptanedioic acid	-4.03	0.0000	0.0000	3645320	223619	annotated
675	S-Propyl-L-cysteine	-1.81	0.0000	0.0000	3074695	878198	annotated+fragment
704	N-gamma-L-Glutamyl-L-methionine	-2.47	0.0000	0.0000	1058447	191359	annotated
712	PC(16:1(9Z)/0:0)	-1.60	0.0000	0.0000	4028181	1331823	annotated
713	N-a-Acetylcitrulline	-2.50	0.0000	0.0000	4325303	763066	annotated
740	Hydroxypropyl-Hydroxyproline	-1.84	0.0000	0.0000	3327208	928317	annotated
746	Alanyl-Proline	-1.01	0.0000	0.0000	3593120	1782045	annotated
767	Midodrine	-1.80	0.0000	0.0000	2972192	853517	annotated
784	Maleamate	-1.87	0.0000	0.0000	1963966	537834	annotated
787	2,3-dihydroxy-valeric acid	-1.87	0.0000	0.0000	258890	70680	annotated

788	Histidinyl-Glycine	-1.14	0.0000	0.0000	3160522	1432470	annotated
804	Ne,Ne dimethyllysine	-2.46	0.0000	0.0000	2170840	393462	annotated
820	(Ac)2-L-Lys-D-Ala	-1.56	0.0000	0.0000	1111400	376353	annotated
881	Isoleucyl-Leucine	-1.53	0.0000	0.0000	1979440	684947	annotated
914	Purine	-4.40	0.0000	0.0000	1188763	56261	annotated+fragment
971	Suberylglycine	-1.51	0.0000	0.0000	1306326	459228	annotated
972	Butabarbital	-2.40	0.0000	0.0000	1228082	231937	annotated
1044	N-Formyl-4-amino-5-aminomethyl-2-methylpyrimidine	-1.18	0.0000	0.0000	1825953	804341	annotated
1132	Methionine sulfoxide	-1.07	0.0000	0.0000	1557792	740741	annotated
1142	Lysyl-Tyrosine	-1.90	0.0000	0.0000	290618	78135	annotated
1175	L-Coprine	-1.54	0.0000	0.0000	1129432	388213	annotated
1216	5,6-Dihydroxyindole	-2.19	0.0000	0.0000	1018771	223706	annotated
1300	Benthiavalicarb isopropyl	-1.86	0.0000	0.0000	106104	29169	annotated
1353	alpha-linolenic acid	-1.76	0.0000	0.0000	790727	234113	annotated
1477	3-Isoxazolidinone	-1.53	0.0000	0.0000	618757	214976	annotated
1549	L-4-Hydroxyglutamine	-1.54	0.0000	0.0000	796846	273245	annotated
1588	O-Desmethylcarvedilol	-2.30	0.0000	0.0000	137896	27935	annotated
1605	Pentostatin	-1.87	0.0000	0.0000	543847	149256	annotated
1691	Metronidazole	-2.13	0.0000	0.0000	498476	113784	annotated
1796	1-Palmitoylglycerophosphoinositol	-1.41	0.0000	0.0000	447744	168312	annotated
1864	Homocysteine	-1.42	0.0000	0.0000	274436	102750	annotated
1865	Dihydro-4-mercapto-3(2H)-furanone	-1.53	0.0000	0.0000	98284	34041	annotated
1873	Dihydrobiopterin	-1.00	0.0000	0.0000	408365	204795	annotated
1878	N-a-Acetyl-L-arginine	-2.08	0.0000	0.0000	368763	86982	annotated
1940	Monuron	-1.14	0.0000	0.0000	304597	138169	annotated
1945	(R)-2-Hydroxysterculic acid	-1.54	0.0000	0.0000	238523	82086	annotated
2120	3-Keto-scylo-inosamine	-1.66	0.0000	0.0000	267910	84746	annotated
2256	Acetylcysteine	-2.13	0.0000	0.0000	129146	29598	annotated
2374	Theasinensin C	-2.67	0.0000	0.0000	161242	25284	annotated

2744	ethyl tetradecanoate	-2.41	0.0000	0.0000	592208880	111697922	annotated
2778	D-chiro-Inositol	-1.36	0.0000	0.0000	169820148	66264313	annotated+fragment
2779	(1R,2R)-3-[(1,2-Dihydro-2-hydroxy-1-naphthalenyl)thio]-2-oxopropanoic acid	-0.90	0.0000	0.0000	793205	424617	annotated
2781	2-(2-Thienylmethylene)-1,6-dioxaspiro[4.4]non-3-ene	-0.99	0.0000	0.0000	423998	213399	annotated
2836	D-Glucono-1,5-lactone	-1.68	0.0000	0.0000	1538292	479312	annotated
2843	D-altro-D-manno-Heptose	-2.86	0.0000	0.0000	475563	65635	annotated
2845	L-Tyrosine	-2.01	0.0000	0.0000	380578	94619	annotated
2850	Aspartyl-Glutamine	-1.90	0.0000	0.0000	264417	70689	annotated
2853	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	-1.66	0.0000	0.0000	194414	61550	annotated
2890	2-Oxoglutaramate	-1.33	0.0000	0.0000	710035	281898	annotated
2913	Alloxanthine	-1.81	0.0000	0.0000	48985366	13998363	annotated+fragment
2923	9-Aminocamptothecin	-1.54	0.0000	0.0000	113761	39070	annotated
2924	L-alpha-glutamyl-L-hydroxyproline	-2.05	0.0000	0.0000	73054	17663	annotated
2927	Asparaginyl-Proline	-1.91	0.0000	0.0000	48330	12857	annotated
2955	Dolichyl phosphate D-mannose	-2.54	0.0000	0.0000	10352389	1780737	annotated+fragment
2956	D-Xylulose 5-phosphate	-1.95	0.0000	0.0000	3062867	790985	annotated
2957	D-Ribulose 5-phosphate	-1.95	0.0000	0.0000	3062867	790985	annotated
2959	5-L-Glutamyl-taurine	-2.43	0.0000	0.0000	2803235	520493	annotated
2962	N-Acetylgalactosamine 6-sulfate	-3.21	0.0000	0.0000	1717310	185421	annotated
2964	Aspartyl-Serine	-2.12	0.0000	0.0000	1219080	280504	annotated
2965	7-Hydroxymethyl-12-methylbenz[a]anthracene sulfate	-2.52	0.0000	0.0000	482662	84431	annotated
2966	D-Glycero-D-galacto-heptitol	-5.97	0.0000	0.0000	370598	5927	annotated
2973	L-N-Carboxymethylserine	-1.42	0.0000	0.0000	180663	67560	annotated
2974	D-Galactonate	-1.37	0.0000	0.0000	38273667	14771917	annotated+fragment
2994	Ovalitenin A	-2.64	0.0000	0.0000	491374	78750	annotated
2998	2'-Deoxysepiapterin	-1.08	0.0000	0.0000	115175	54498	annotated
3005	3-Phospho-DL-glycerate	-3.10	0.0000	0.0000	7265401	848568	annotated+fragment
3006	Triphenylsilanol	-2.52	0.0000	0.0000	1400530	244909	annotated+fragment
3045	Uracil	-1.44	0.0000	0.0000	14769556	5448628	annotated

3046	Potassium 2-(1'-ethoxy) ethoxypropanoate	-2.80	0.0000	0.0000	5250992	756480	annotated
3057	D-Ribonate	-1.27	0.0000	0.0000	2881534	1196009	annotated
3058	1-Isothiocyanato-7-(methylsulfinyl)heptane	-1.28	0.0000	0.0000	312673	128575	annotated
3065	(x)-1,2-Propanediol 1-O-b-D-glucopyranoside	-3.88	0.0000	0.0000	1488178	100948	annotated
3069	5'-Dehydroadenosine	-2.77	0.0000	0.0000	164345	24158	annotated
3084	1-Stearoylglycerophosphoinositol	-1.59	0.0000	0.0000	1649393	548185	annotated+fragment
3108	Egonol	-2.07	0.0000	0.0000	131636	31427	annotated
3109	omega-Hydroxymoracin N	-2.07	0.0000	0.0000	131636	31427	annotated
3138	L-Aspartyl-L-phenylalanine	-2.12	0.0000	0.0000	89897	20750	annotated
3139	Sedoheptulose 1-phosphate	-3.51	0.0000	0.0000	11393206	997401	annotated+fragment
3142	Threonic acid	-1.54	0.0000	0.0000	11127084	3826366	annotated
3179	Xanthosine	-2.69	0.0000	0.0000	1258177	194654	annotated+fragment
3256	Salsoline-1-carboxylate	-1.99	0.0000	0.0000	978907	245750	annotated
3257	Phenylpropionylglycine	-2.19	0.0000	0.0000	885904	194454	annotated
3269	6,7-Benzocoumarin	-1.78	0.0000	0.0000	194509	56444	annotated
3276	11-Eicosenoic acid	-2.53	0.0000	0.0000	4931082	854253	annotated
3280	(S)-3-Hydroxybutanoate	-1.82	0.0000	0.0000	6669504	1889062	annotated
3293	Glycerophosphoglycerol	-1.49	0.0000	0.0000	4561918	1628628	annotated
3342	Ethylphosphate	-3.52	0.0000	0.0000	4251178	370249	annotated
3355	Quercetin 3-(2"-galloyl-alpha-L-arabinopyranoside)	#NUM!	0.0000	0.0000	72169	0	annotated
3379	Glycyl-Asparagine	-1.72	0.0000	0.0000	137641	41712	annotated
3384	Nocardicin F	-1.43	0.0000	0.0000	180207	66991	annotated
3416	5-Oxoavermectin "2a" aglycone	-1.77	0.0000	0.0000	3330946	974741	annotated+fragment
3436	sn-Glycero-3-phospho-1-inositol	-2.44	0.0000	0.0000	4318326	797905	annotated
3476	Monoethyl malonic acid	1.94	0.0000	0.0000	354413	1363763	annotated+fragment
3482	L-Arabinose	-2.12	0.0000	0.0000	2886237	662479	annotated
3483	beta-D-Glucosamine	-1.14	0.0000	0.0000	2181872	988276	annotated
3484	Methyl 1-(propylsulfinyl)propyl disulfide	-1.78	0.0000	0.0000	259032	75628	annotated
3522	N-Acetyl-alpha-D-galactosamine 1-phosphate	-2.10	0.0000	0.0000	1982767	462232	annotated

3543	(all-E)-1,7-bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-one	-2.25	0.0000	0.0000	146992	30974	annotated
3553	PE(18:1(9Z)/0:0)	-2.01	0.0000	0.0000	2169480	540353	annotated
3561	D-Biopterin	-1.79	0.0000	0.0000	141454	40990	annotated
3725	Dambonitol	-4.05	0.0000	0.0000	974900	58661	annotated
3833	N-Acetyl-L-methionine	-1.93	0.0000	0.0000	632629	165690	annotated
4043	Pyrocatechol sulfate	-1.74	0.0000	0.0000	568601	170148	annotated
4045	4-[2-(5-Carboxy-2-hydroxy-3-methoxyphenyl)-2-oxoethylidene]-2-hydroxy-2-pentenedioate	-3.17	0.0000	0.0000	152323	16926	annotated
4050	SB 206553	-0.25	0.0000	0.0000	111390	93404	annotated
4082	Tauropine	-1.75	0.0000	0.0000	391945	116503	annotated
4388	Danthron	-2.01	0.0000	0.0000	410820	102037	annotated
4522	2-O-beta-D-Glucopyranuronosyl-D-mannose	-1.77	0.0000	0.0000	310780	90868	annotated
4680	Asparaginyln-Gamma-glutamate	-1.41	0.0000	0.0000	77472	29066	annotated
4686	Maltopentaose	-2.90	0.0000	0.0000	174884	23373	annotated
4739	1-O-Methyl-myo-inositol	-1.35	0.0000	0.0000	246854	96914	annotated
4954	Sulforaphane-N-acetylcysteine	-1.56	0.0000	0.0000	187428	63708	annotated
5274	Eriojaposide A	-1.18	0.0000	0.0000	92957	40892	annotated
5490	Hirsutin	-1.08	0.0000	0.0000	57328	27040	annotated
97	Phensuximide	-1.50	0.0000	0.0001	651208	230516	annotated
99	Coformycin	-1.52	0.0000	0.0001	287915	100318	annotated
199	3-Acetylthiophene	-1.18	0.0000	0.0001	425834	188159	annotated
218	Hydroxypropyl-Arginine	-2.11	0.0000	0.0001	468450	108163	annotated
220	Glycyl-Glutamine	-1.13	0.0000	0.0001	455091	207721	annotated
230	Nalbuphine	-1.07	0.0000	0.0001	718058	340961	annotated
242	N-Methylnicotinate	-1.30	0.0000	0.0001	37472630	15197452	annotated+fragment
270	Glycyl-Lysine	-2.31	0.0000	0.0001	332447	67212	annotated
424	N6-Methyladenosine	-1.92	0.0000	0.0001	468872	124047	annotated
27	Choline phosphate	-0.91	0.0000	0.0001	405994096	215471644	identified
609	Cohibin C	-0.72	0.0000	0.0001	4424735	2684138	annotated
634	Didodecyl thiobispropanoate	1.47	0.0000	0.0001	1517503	4197526	annotated

3801	2-Oxoglutarate	1.48	0.0000	0.0001	621631	1739905	identified
4241	cis-Aconitate	-1.53	0.0000	0.0001	228688	79253	identified
707	3'-O-Methylguanosine	-1.24	0.0000	0.0001	391717	165728	annotated+fragment
708	1-Methylguanosine	-1.24	0.0000	0.0001	391717	165728	annotated+fragment
868	L-Histidine trimethylbetaine	-1.18	0.0000	0.0001	1988405	875915	annotated
876	Carboxy-ibuprofen	1.46	0.0000	0.0001	949306	2620542	annotated
877	2,3-Dehydrosalvipisone	1.37	0.0000	0.0001	253220	654977	annotated
896	Phosphodimethylethanolamine	-1.16	0.0000	0.0001	1565251	700993	annotated
1071	Nicotinamide D-ribonucleotide	-1.39	0.0000	0.0001	1571447	597818	annotated+fragment
1464	Clobenpropit	-1.14	0.0000	0.0001	777691	353919	annotated
1489	Arginyl-Proline	-1.64	0.0000	0.0001	559077	179205	annotated
1516	PC(14:0/0:0)	-1.13	0.0000	0.0001	741517	339849	annotated
1542	Butalbital	-1.07	0.0000	0.0001	618258	295070	annotated
1550	Glycyl-Serine	-1.13	0.0000	0.0001	597863	273067	annotated
1574	Chitobiose	-1.71	0.0000	0.0001	548185	167809	annotated
1617	FPL64176	-1.89	0.0000	0.0001	495049	133521	annotated
1713	Protoanemonin	-1.19	0.0000	0.0001	469002	206071	annotated
1937	S-Acetylphosphopantetheine	-3.04	0.0000	0.0001	255243	31113	annotated
1950	Diisopropyl sulfate	-1.26	0.0000	0.0001	248355	103861	annotated
2236	3R-aminononanoic acid	-1.22	0.0000	0.0001	157146	67286	annotated
2419	5-Phosphonoxy-L-lysine	-1.28	0.0000	0.0001	105212	43413	annotated
2434	Glucosylisomaltol	-1.38	0.0000	0.0001	120347	46159	annotated
2762	trans-Cinnamate	-1.64	0.0000	0.0001	398945	127828	annotated
2806	Levoglucofan	-1.59	0.0000	0.0001	3925474	1305274	annotated
2807	3-Ureidopropionate	-0.99	0.0000	0.0001	4053772	2046393	annotated
2808	3E-methylglutaconic acid	-1.35	0.0000	0.0001	2329024	916155	annotated
2809	4,4'-Sulfonyldiphenol	-1.35	0.0000	0.0001	1863204	730538	annotated
2815	beta-L-Arabinofuranose	-1.39	0.0000	0.0001	551876	210725	annotated
2847	Aminofructose 6-phosphate	-1.29	0.0000	0.0001	433410	176638	annotated
2856	Pyroglutamylglycine	-1.15	0.0000	0.0001	98116	44144	annotated

2903	PC(O-2:0/O-2:0)	-2.17	0.0000	0.0001	45756	10158	annotated
2919	Oroselone	-2.01	0.0000	0.0001	165647	41085	annotated
3014	N-Succinyl-2-L-amino-6-oxoheptanedioate	1.49	0.0000	0.0001	277813	778737	annotated
3129	Pseudouridine	-0.85	0.0000	0.0001	17651708	9783181	annotated+fragment
3173	(Z,Z)-2-Methyl-5-(8,11,14-pentadecatrienyl)-1,3-benzenediol	-2.34	0.0000	0.0001	8665629	1710397	annotated
3196	Cer(d18:1/22:1(13Z))	-1.30	0.0000	0.0001	146166	59457	annotated
3271	a-Methyldopa mono-O-sulfate	-1.69	0.0000	0.0001	54158	16741	annotated
3372	Mannitol	-2.65	0.0000	0.0001	2808482	446243	annotated
3555	Demeton-O	-1.96	0.0000	0.0001	1721019	442191	annotated
3660	Linoleic acid	-1.75	0.0000	0.0001	1276956	380028	annotated
3704	Myristicin	-1.56	0.0000	0.0001	20472	6940	annotated
3800	2-O-Benzoyl-D-glucose	-3.17	0.0000	0.0001	1008380	112030	annotated
3958	(-)-1-Methylpropyl 1-propenyl disulfide	-1.14	0.0000	0.0001	878457	397323	annotated+fragment
4064	S-Nitrosoglutathione	-1.66	0.0000	0.0001	520942	164542	annotated
4236	L-phenylalanyl-L-hydroxyproline	-1.80	0.0000	0.0001	382678	110203	annotated
4701	Glycyl-Tryptophan	-1.52	0.0000	0.0001	67413	23486	annotated
4743	2-Methylcitric acid	-1.22	0.0000	0.0001	228110	98132	annotated
5240	Didanosine	-1.51	0.0000	0.0001	108309	37939	annotated
11	2-Acetylpyrazine	-0.68	0.0000	0.0002	1322406784	826898112	annotated+fragment
62	5-Hydroxyindoleacetate	-1.29	0.0000	0.0002	712631	291580	annotated
144	2-O-(6-Phospho-alpha-mannosyl)-D-glycerate	-1.54	0.0000	0.0002	4209658	1447334	annotated+fragment
161	PC(16:0/0:0)	-0.97	0.0000	0.0002	100852696	51348146	annotated
273	Mefenacet	-2.12	0.0000	0.0002	211969	48696	annotated
1085	Phytosphingosine	-0.79	0.0000	0.0002	1530889	884704	annotated
225	L-Lysine	-1.42	0.0000	0.0002	43407129	16207801	identified+fragment
1114	riboflavin	-1.25	0.0000	0.0002	1078849	454554	identified+fragment
1692	3-Hydroxystigmast-5-en-7-one	-1.60	0.0000	0.0002	382024	125860	annotated
1818	Dimorphecolic acid	-1.17	0.0000	0.0002	376440	167513	annotated
2086	2-Hydroxy-3-methyl-9H-carbazole	-1.15	0.0000	0.0002	30103	13595	annotated

2245	(6RS)-6,19-epidioxy-24,24-difluoro-25-hydroxy-6,19-dihydrovitamin D3 / (6RS)-6,19-epidioxy-24,24-difluoro-25-hydroxy-6,19-dihydrocholecalciferol	-1.01	0.0000	0.0002	190038	94146	annotated
2505	Normetanephrine	-0.75	0.0000	0.0002	106185	63316	annotated
3047	Homocysteinesulfinic acid	-1.19	0.0000	0.0002	1699994	743049	annotated
3168	Clidinium	-1.36	0.0000	0.0002	29843	11636	annotated
3284	PI(18:1(9Z)/18:2(9Z,12Z))	-0.96	0.0000	0.0002	5701845	2937841	annotated
3414	1-Deoxy-D-altro-heptulose 7-phosphate	-1.76	0.0000	0.0002	1966867	579891	annotated
3719	Ethyl glucuronide	-2.57	0.0000	0.0002	1394777	234392	annotated
4084	Ethyl 2-hydroxyisovalerate	-0.96	0.0000	0.0002	453230	233659	annotated
4218	Phenindione	-2.35	0.0000	0.0002	378909	74526	annotated
4292	PE(22:5(7Z,10Z,13Z,16Z,19Z)/14:0)	-0.90	0.0000	0.0002	491275	263237	annotated
4855	D-Glucose 6-sulfate	-2.52	0.0000	0.0002	145031	25212	annotated
139	Isoleucyl-Aspartate	-1.33	0.0001	0.0003	891085	353830	annotated+fragment
443	S-Prenyl-L-cysteine	-1.44	0.0001	0.0003	7260942	2685103	annotated
917	2-Methoxyestradiol-17beta 3-sulfate	-1.45	0.0001	0.0003	80935	29658	annotated
1518	Allocystathionine	-2.44	0.0001	0.0003	474422	87353	annotated+fragment
693	Cytidine	-1.32	0.0000	0.0003	3255725	1304475	identified
2126	N-Methylcalystegine C1	-0.94	0.0001	0.0003	214352	111983	annotated
2215	Isocarbamid	-1.24	0.0001	0.0003	199179	84097	annotated
2446	1-Methylseleno-N-acetyl-D-galactosamine	-3.19	0.0001	0.0003	89774	9866	annotated
2616	Acetoxyacetone	-1.34	0.0001	0.0003	64975	25710	annotated
3062	Urolithin B	-1.28	0.0001	0.0003	94348	38894	annotated
3894	Methyl benzoate	0.99	0.0001	0.0003	617436	1222697	annotated
4389	Monomethyl sulfate	-1.42	0.0000	0.0003	448437	167457	annotated
4580	Sulfamoyldapsone	0.83	0.0001	0.0003	234733	417073	annotated
319	Histidinyl-Serine	-1.30	0.0001	0.0004	2487892	1008785	annotated+fragment
346	Ophthalmic acid	1.52	0.0001	0.0004	3641704	10426950	annotated+fragment
1176	Histidinyl-Asparagine	-1.18	0.0001	0.0004	615300	270992	annotated
1316	Methomyl	-1.06	0.0001	0.0004	871100	417776	annotated

1779	1-Oleoylglycerophosphoserine	-0.90	0.0001	0.0004	439048	235264	annotated
2252	Deoxyinosine	-1.16	0.0001	0.0004	105325	47245	annotated
2388	N-(1-Deoxy-1-fructosyl)tyrosine	-3.54	0.0001	0.0004	142272	12258	annotated
2451	N-lactoyl-Tryptophan	-1.28	0.0001	0.0004	73111	30079	annotated
3083	Fexofenadine	-1.65	0.0001	0.0004	2333890	745101	annotated
3127	Tyramine	-1.35	0.0001	0.0004	69020	27036	annotated
3145	(1R,2S)-1-Hydroxypropane-1,2,3-tricarboxylate	-1.85	0.0001	0.0004	3398344	941903	annotated
3148	Propane-1,2-diol 1-phosphate	-2.31	0.0001	0.0004	349162	70338	annotated
3219	Propionic acid	-2.19	0.0001	0.0004	6293783	1381089	annotated+fragment
4032	5-Hydroxymethyl-2-furaldehyde	-1.28	0.0001	0.0004	628501	258032	annotated
4282	Oxalosuccinate	0.98	0.0001	0.0004	201918	399621	annotated
4464	Epoxiconazole	2.12	0.0001	0.0004	59835	259410	annotated
262	cis-3-Hexenyl b-primeveroside	-2.58	0.0001	0.0005	132647	22171	annotated
426	N6,N6,N6-Trimethyl-L-lysine	-1.52	0.0001	0.0005	7740261	2703394	annotated+fragment
1207	7-Aminomethyl-7-carbaguanine	-1.21	0.0001	0.0005	118691	51163	annotated
1367	L-glycyl-L-hydroxyproline	-0.96	0.0001	0.0005	532438	273131	annotated
1554	Asparaginy-L-Histidine	-1.18	0.0001	0.0005	615300	270992	annotated
1699	Ethoxzolamide	-1.30	0.0001	0.0005	236352	95818	annotated
2441	xi-4,5-Dihydro-2,4(5)-dimethyl-1H-imidazole	-1.45	0.0001	0.0005	78098	28496	annotated
60	L-Kynurenine	-1.34	0.0001	0.0005	2848111	1127072	identified+fragment
3143	Isocitrate	-1.83	0.0001	0.0005	3398344	957059	annotated
3278	5-Hydroxy-7-tetracosanone	-1.47	0.0001	0.0005	454546	163577	annotated
4024	PG(18:2(9Z,12Z)/0:0)	-0.99	0.0001	0.0005	220457	110931	annotated
4194	3-oxo-tetradecanoic acid	-1.49	0.0001	0.0005	243827	86766	annotated
4379	Indolelactate	-1.40	0.0001	0.0005	192361	73064	annotated
55	gamma-L-Glutamyl-L-cysteine	-0.65	0.0001	0.0006	2686568	1709847	annotated+fragment
140	Tos-Arg-CH2Cl	-1.58	0.0001	0.0006	618857	206835	annotated
224	3beta,6beta-Dihydroxynortropane	-0.91	0.0001	0.0006	40499404	21512817	annotated
791	Oxidized glutathione	-1.37	0.0001	0.0006	1652446	639971	annotated+fragment
1401	PS(O-16:0/20:1(11Z))	-1.82	0.0001	0.0006	746163	211700	annotated

1486	Lysyl-Serine	-2.17	0.0001	0.0006	434905	96408	annotated
1656	2-Methylaminoadenosine	-1.32	0.0001	0.0006	334003	134080	annotated
3538	N-lactoyl-Methionine	-2.26	0.0001	0.0006	1233730	258153	annotated
3602	Quinoline yellow	-0.98	0.0001	0.0006	184403	93807	annotated
4262	Ipomeatetrahydrofuran	1.07	0.0001	0.0006	250796	527989	annotated
4742	S-Propyl 2-propene-1-sulfinothioate	-0.99	0.0001	0.0006	234920	118060	annotated
5017	Beta-Citryl-L-glutamic acid	-1.23	0.0001	0.0006	100176	42804	annotated
5497	Ikarisoside A	2.31	0.0001	0.0006	12527	61945	annotated
648	N-Formimino-L-glutamate	2.46	0.0002	0.0007	242114	1334543	annotated
1403	p-Hydroxyfelbamate	-1.53	0.0002	0.0007	837326	290786	annotated
3123	Fosamine	-0.98	0.0002	0.0007	335306	169879	annotated
4806	Sphingosine 1-phosphate	0.82	0.0002	0.0007	72546	127680	annotated
5340	lipoamide	-0.84	0.0002	0.0007	92880	51934	annotated
292	PE(20:4(5Z,8Z,11Z,14Z)/0:0)	-1.57	0.0002	0.0008	3715974	1251835	annotated
1028	5-Methylthio-D-ribose	-0.80	0.0002	0.0008	1771113	1018988	annotated
1313	Hypotaurocyamine	-1.58	0.0002	0.0008	657686	219976	annotated
2197	Hydroxypropyl-Glutamine	-1.45	0.0002	0.0008	163985	60085	annotated
2801	Taurine	-0.67	0.0002	0.0008	104988204	65820270	identified+fragment
2929	Urate	-0.75	0.0002	0.0008	35890126	21321498	annotated
2990	L-beta-aspartyl-L-glutamic acid	-1.14	0.0002	0.0008	84367	38345	annotated
3039	Xanthosine 5'-phosphate	-0.86	0.0002	0.0008	1860878	1022866	annotated
3081	Sulfinpyrazone	-5.24	0.0002	0.0008	81087	2144	annotated
3383	desbutyl-lumefantrine	-1.23	0.0002	0.0008	270983	115198	annotated
3486	Phenylpropanoate	-2.12	0.0002	0.0008	1533153	351753	annotated
3991	Glycerone phosphate	-1.31	0.0002	0.0008	326785	131749	annotated
4044	D-Erythrose 4-phosphate	-1.52	0.0002	0.0008	255973	89554	annotated
4277	Nevirapine	0.73	0.0002	0.0008	278014	462301	annotated
4554	a-L-threo-4-Hex-4-enopyranuronosyl-D-galacturonic acid	0.98	0.0002	0.0008	67324	132917	annotated
275	N,N'-Diacetylhydrazine	-0.93	0.0002	0.0009	101651	53372	annotated

314	Isoleucyl-Alanine	-1.38	0.0002	0.0009	17976014	6905190	annotated
375	Thiomorpholine 3-carboxylate	-1.43	0.0002	0.0009	6577523	2441943	annotated
1560	Etorphine	-1.14	0.0002	0.0009	692509	313862	annotated
2025	Isonicotinic acid	-0.88	0.0002	0.0009	226243	123112	annotated
3274	IMP	-1.31	0.0002	0.0009	6410423	2588438	annotated+fragment
3341	Ethyl hydrogen sulfate	-1.36	0.0002	0.0009	4490641	1754570	annotated
3487	3-Succinoylpyridine	-3.09	0.0002	0.0009	292052	34385	annotated
3738	3,4-Dihydroxyphenylpropanoate	-1.55	0.0002	0.0009	1424009	486636	annotated+fragment
5436	3-Methoxy-4,5-methylenedioxycinnamaldehyde	-2.33	0.0002	0.0009	29404	5867	annotated
2773	Pentobarbital	-2.04	0.0002	0.0010	222831316	54342057	annotated
2938	Sulfate	-3.10	0.0002	0.0010	20754201	2424490	annotated
4856	Apigenin 7-sulfate	-1.54	0.0003	0.0010	117649	40354	annotated
5194	Polyethylene, oxidized	-0.66	0.0003	0.0010	109413	69021	annotated
747	Histidinyl-Threonine	-0.93	0.0003	0.0011	1732328	909116	annotated
2445	N4-Acetylcytidine	-0.84	0.0003	0.0011	101343	56707	annotated
3908	Methionyl-Methionine	-1.91	0.0003	0.0011	36906	9796	annotated
5220	CDP-ribitol	0.88	0.0003	0.0011	66182	121657	annotated
285	LysoPC(20:3(5Z,8Z,11Z))	-1.52	0.0003	0.0012	480952	167407	annotated
309	N-Palmitoylsphingosine	-0.83	0.0003	0.0012	23899811	13418718	annotated
1151	(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	-0.79	0.0003	0.0012	1195941	692908	annotated
2033	S-Propyl thiosulfate	1.72	0.0003	0.0012	56868	187788	annotated
2947	Trimetaphosphoric acid	-1.75	0.0003	0.0012	285906	84963	annotated
3214	Hexamethylene bisacetamide	-1.39	0.0003	0.0012	9901956	3773295	annotated
3713	D-Glucuronic acid	-0.85	0.0003	0.0012	1421760	790389	annotated+fragment
3892	3-Ethenyl-2,5-dimethyl-4-oxohex-5-en-2-yl acetate	-0.90	0.0003	0.0012	365350	195760	annotated
3893	Jasmonic acid	-0.90	0.0003	0.0012	365350	195760	annotated
4367	N-Acetoxy-IQ	-0.87	0.0003	0.0012	396675	216291	annotated
4422	Ethyl 1-(ethylthio)propyl disulfide	-1.26	0.0003	0.0012	148454	61899	annotated
96	Glutamylphenylalanine	-1.04	0.0003	0.0013	1566838	760125	annotated

1874	L-2-Aminoethyl seryl phosphate	-1.06	0.0003	0.0013	281031	134779	annotated
2073	Clitidine	-1.59	0.0003	0.0013	217696	72304	annotated
2878	Cycloprothrin	-1.16	0.0003	0.0013	174896	78242	annotated
202	N-Butyryl-L-homoserine lactone	-1.38	0.0004	0.0014	211677	81412	annotated
329	N2,N2-Dimethylguanosine	-0.97	0.0004	0.0014	263583	134936	annotated
456	Hydroxypropionylcarnitine	-1.53	0.0004	0.0014	974414	336415	annotated
2270	Prunetin	-0.90	0.0004	0.0014	166748	89090	annotated
3132	Ezetimibe	-1.00	0.0004	0.0014	969933	483488	annotated
639	O-Propanoylcarnitine	1.58	0.0004	0.0015	865905	2585354	annotated
715	Valerylglycine	-0.96	0.0004	0.0015	2521886	1296011	annotated
2864	(Z)-But-1-ene-1,2,4-tricarboxylate	-0.90	0.0004	0.0015	231282	123909	annotated
3175	PG(18:1(9Z)/0:0)	-1.52	0.0004	0.0015	534921	186166	annotated
287	PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	-2.79	0.0004	0.0016	262580	37913	annotated
1496	PG(18:4(6Z,9Z,12Z,15Z)/0:0)	-1.63	0.0004	0.0016	131556	42632	annotated
517	Hypotaurine	-0.86	0.0005	0.0017	7442742	4102971	annotated
2486	L-Formylkynurenine	-0.94	0.0005	0.0017	85827	44678	annotated
3012	Isosyringinoside	1.86	0.0005	0.0017	425437	1540971	annotated
503	alpha-Methylstyrene	-2.13	0.0005	0.0018	4415357	1011401	annotated
1905	1-Pyrroline	-0.74	0.0005	0.0018	293835	176328	annotated
2327	CL(1'-[18:2(9Z,12Z)/0:0],3'-[18:2(9Z,12Z)/0:0])	-3.86	0.0005	0.0018	92293	6373	annotated
2904	Pyrrolidonecarboxylic acid	-1.07	0.0005	0.0018	32366097	15460769	annotated+fragment
4253	1-Acetylcyclohexyl acetate	-0.81	0.0005	0.0018	457502	261837	annotated
4898	2',3'-Cyclic UMP	-1.71	0.0005	0.0018	137330	41907	annotated
306	Sulforhodamine B	0.94	0.0005	0.0019	242480	463941	annotated
1780	L-Cystine	-3.25	0.0005	0.0019	301284	31620	identified
4033	D-Glucosamine	-0.94	0.0005	0.0019	137594	71710	identified
5007	Dihydro-2,4-dimethyl-6-(2-methylpropyl)-4H-1,3,5-dithiazine	-0.61	0.0005	0.0019	128656	84200	annotated
435	Orthophosphate	-0.66	0.0006	0.0020	10102173	6407204	annotated
1029	Hydroxypropyl-Leucine	-1.34	0.0005	0.0020	1560215	615236	annotated

2820	5-Hydroxy-2-furoic acid	-0.94	0.0005	0.0020	156865	81890	annotated
4007	3-keto-n-caprylic acid	-0.74	0.0006	0.0020	977706	585199	annotated
2136	Thiophene	-1.58	0.0006	0.0021	146226	48935	annotated
2473	8-Oxodeoxycoformycin	-0.88	0.0006	0.0021	89898	48790	annotated
1045	Isoputreanine	-1.33	0.0006	0.0022	1319335	526175	annotated+fragment
2232	S-Cysteinossuccinic acid	-1.00	0.0006	0.0022	61240	30629	annotated
2922	2-Protocatechloylphloroglucinolcarboxylate	-1.24	0.0006	0.0022	69226	29349	annotated
3125	Dihydrogen phosphate	-0.86	0.0006	0.0022	262433	145076	annotated
711	S-3-oxodecanoyl cysteamine	-1.49	0.0007	0.0023	2972454	1055533	annotated
1627	3-keto palmitic acid	-2.09	0.0006	0.0023	348809	81858	annotated
3656	1-Pyrroline-5-carboxylic acid	-1.50	0.0007	0.0023	469952	165753	annotated
5410	3-hydroxy-undecanoic acid	-0.68	0.0006	0.0023	82648	51648	annotated
163	L-Pipecolate	-1.18	0.0007	0.0024	13576822	5975548	annotated
1122	Sodium sulfate	-1.07	0.0007	0.0024	1278330	606989	annotated
3509	Phenylacetic acid	1.01	0.0007	0.0024	1443888	2910782	annotated
221	Eplerenone	-2.35	0.0007	0.0025	26653823	5239831	annotated
948	Pirbuterol	-0.91	0.0007	0.0025	1367350	726744	annotated
1032	Aspartyl-Threonine	-1.01	0.0007	0.0025	1083519	536987	annotated
2144	N-Nitrosodiethylamine	-0.98	0.0007	0.0025	168172	85432	annotated
3446	4,4'-Thiodianiline	-1.22	0.0007	0.0025	33154	14259	annotated
117	N-Alpha-acetyllysine	-1.26	0.0008	0.0026	10940762	4558423	annotated+fragment
4291	PA(18:2(9Z,12Z)/0:0)	-0.86	0.0007	0.0026	414060	227716	annotated
4442	Quercetin 3-xylosyl-(1->6)-glucoside	2.23	0.0007	0.0026	16377	76795	annotated
823	5,6-Dihydrothymine	-0.60	0.0008	0.0028	3471208	2285297	annotated
3194	Cer(d18:0/16:0)	-1.20	0.0009	0.0029	810230	352370	annotated
2872	CMP-N-acetylneuraminic acid	-0.76	0.0009	0.0030	101458	60062	annotated
1924	Epicatechin 5-O-beta-D-glucopyranoside-3-benzoate	1.40	0.0009	0.0031	143225	378825	annotated
2014	Malonylcarnitine	-0.76	0.0010	0.0033	226865	133781	annotated
4392	Mandelonitrile sophoroside	1.36	0.0010	0.0033	89195	228603	annotated
3222	2,5-Dimethyl-3-(methylthio)furan	-2.29	0.0010	0.0034	1139158	233009	annotated

4175	xi-2,2,6-Trimethyl-1,4-cyclohexanedione	-0.45	0.0010	0.0034	377421	276926	annotated
5423	Quinaprilat	-1.15	0.0010	0.0034	52529	23614	annotated
878	Nafenopin	1.55	0.0011	0.0035	224090	654977	annotated
1433	PS(18:0/0:0)	-0.75	0.0011	0.0035	834955	497550	annotated
1746	Galactosylhydroxylysine	-1.15	0.0011	0.0035	348830	156840	annotated
4039	3-Sulfinoalanine	-3.01	0.0011	0.0035	214199	26532	annotated
1006	Adenylsuccinic acid	1.60	0.0011	0.0036	315759	954097	annotated+fragment
3153	N-(1-Deoxy-1-fructosyl)threonine	-2.90	0.0011	0.0036	57930	7735	annotated
4848	Valaciclovir	-1.07	0.0011	0.0036	159888	75934	annotated
1970	4-Pyridoxate	-1.16	0.0012	0.0037	201696	89952	annotated
2937	PI(18:1(9Z)/18:1(11Z))	-1.42	0.0012	0.0037	561534	210318	annotated
3177	7,9-Tetracosanedione	-1.26	0.0012	0.0037	272615	113897	annotated
3880	Dephospho-CoA	-2.36	0.0012	0.0037	575819	112288	annotated
4171	Polypropylene glycol (m w 1,200-3,000)	-1.82	0.0011	0.0037	240522	68081	annotated
179	PE(22:1(13Z)/15:0)	-0.49	0.0012	0.0038	74578100	53243842	annotated
1786	Tranexamic acid	-0.77	0.0012	0.0038	289194	169633	annotated
1487	N-Methylhistamine	-1.69	0.0012	0.0039	320395	99194	annotated
4955	Patulin	-0.59	0.0012	0.0039	149927	99299	annotated
604	Succinyladenosine	-0.73	0.0013	0.0041	5667656	3428374	annotated
3178	D-Glycerate	-1.32	0.0013	0.0041	4621225	1851505	annotated+fragment
1583	L-Cysteine	-1.34	0.0013	0.0042	199630	79036	annotated
3344	3-Deoxy-D-manno-octulosonate 8-phosphate	-5.25	0.0013	0.0042	140556	3695	annotated
5363	(3xi,6xi)-Cyclo(alanylvalyl)	-0.73	0.0013	0.0042	85184	51340	annotated
879	N-Jasmonoyltyrosine	1.58	0.0015	0.0045	200133	598189	annotated
3032	Norambreinolide	-1.34	0.0015	0.0045	616103	243072	annotated
4085	Lumichrome	-1.50	0.0014	0.0045	341017	120761	annotated
1165	Histidiny-Tyrosine	-0.82	0.0016	0.0048	372312	211536	annotated
3390	D-4'-Phosphopantothenate	-1.08	0.0015	0.0048	2760166	1308519	annotated
4462	Quinolate	-0.94	0.0015	0.0048	334988	175084	annotated
4901	6,8-Di-O-methylaverufin	-0.91	0.0016	0.0048	68479	36547	annotated

2335	1,4-Diamino-2-nitrobenzene	-0.81	0.0016	0.0049	124512	70970	annotated
4399	N-Lactoyl ethanolamine phosphate	-0.87	0.0016	0.0049	372651	203255	annotated
418	Chrycolide	-1.18	0.0016	0.0050	81859	36107	annotated
4692	Glucosamine 6-sulfate	-1.57	0.0016	0.0050	151223	50794	annotated
2564	4-Methoxybenzyl butanoate	-0.81	0.0017	0.0051	86141	49062	annotated
5015	Diethyl sulfate	-1.59	0.0017	0.0051	132656	44136	annotated
1068	N2-Fructopyranosylarginine	-3.95	0.0017	0.0052	702658	45540	annotated
3971	5-Sulfoxymethylfurfural	-0.94	0.0017	0.0052	716737	372960	annotated
5475	Fukiic acid	-1.07	0.0017	0.0052	42708	20308	annotated
4881	Enalaprilate	-2.49	0.0017	0.0053	42845	7637	annotated
129	Hydroxypropyl-Proline	-0.82	0.0018	0.0055	1741632	986732	annotated
277	Adenine	-0.65	0.0019	0.0058	32470894	20649249	identified+fragment
2999	hexyl propionate	-0.65	0.0020	0.0059	31442355	20010763	annotated
162	PC(18:3(6Z,9Z,12Z)/0:0)	-0.88	0.0020	0.0060	1031276	561221	annotated
988	Gamma-glutamyl-Threonine	-0.92	0.0020	0.0060	676470	357346	annotated
2790	Galactaric acid	-0.72	0.0020	0.0061	1138928	689972	annotated
4164	Glycerol 1,2-cyclic phosphate	-1.00	0.0022	0.0065	340358	170307	annotated
798	LysoPC(20:4(8Z,11Z,14Z,17Z))	-1.90	0.0024	0.0069	1872712	502959	annotated
505	Nonivamide	-1.21	0.0024	0.0070	3073320	1332412	annotated
3408	4-Hydroxychalcone	-1.07	0.0024	0.0071	64537	30703	annotated
1164	Glycyl-Tyrosine	-0.88	0.0025	0.0073	1115859	606265	annotated
3051	Dihydro-4,6-dimethyl-2-(1-methylethyl)-4H-1,3,5-dithiazine	-0.92	0.0025	0.0073	167493	88379	annotated
3198	Chloroform	0.33	0.0025	0.0073	12644282	15945821	annotated
1307	11-amino-undecanoic acid	-1.30	0.0026	0.0074	338756	137627	annotated
4513	Azelaic acid	-0.70	0.0026	0.0074	341579	209893	annotated
1157	Histidinyl-Glutamine	-0.89	0.0026	0.0075	580078	313013	annotated
607	Glycidyl oleate	-0.55	0.0026	0.0076	5807191	3963073	annotated
4911	Vulgarole	-0.71	0.0027	0.0076	157965	96488	annotated
128	L-Glutamate	-0.51	0.0028	0.0079	99882658	69948984	identified+fragment

3160	6-Hydroxy-2-bornanone glucoside	-1.60	0.0028	0.0080	39403	13012	annotated
294	Ectoine	-0.64	0.0029	0.0082	25287251	16223372	annotated+fragment
2584	Dihydro-3(2H)-thiophenone	-0.58	0.0029	0.0082	69159	46144	annotated
3860	Pantetheine 4'-phosphate	-2.57	0.0029	0.0083	985738	166276	annotated
4842	1-(5'-Phosphoribosyl)-5-amino-4-imidazolecarboxamide	-0.48	0.0029	0.0083	168961	121170	annotated
4048	Undecylic acid	-0.64	0.0029	0.0084	715496	460090	annotated+fragment
3244	6-bromo-eicosa-5E,9Z-dienoic acid	-1.72	0.0030	0.0085	41265	12538	annotated
2268	Dihydrozeatin riboside	-1.16	0.0030	0.0086	93479	41781	annotated
1760	Diethanolamine	-0.98	0.0031	0.0088	403362	205036	annotated
5455	Picolinoylglycine	-0.67	0.0032	0.0089	60521	37910	annotated
2867	sn-Glycerol 3-phosphate	-0.50	0.0032	0.0090	63774826	45164426	identified+fragment
1067	delta-Guanidinovaleric acid	-1.12	0.0033	0.0091	587165	269542	annotated
1527	Gamma-glutamyl-Valine	-1.15	0.0033	0.0092	591876	267626	annotated
2196	(2S,2'S)-Pyrosaccharopine	0.77	0.0033	0.0092	40039	68120	annotated
2862	Cinnamyl benzoate	-1.23	0.0033	0.0093	438444	186555	annotated
1359	1-(2H-1,3-Benzodioxol-5-yl)-2-[2,6-dimethoxy-4-(prop-2-en-1-yl)phenoxy]propyl acetate	-1.21	0.0034	0.0095	77080	33417	annotated
1129	N-Despyridinyl rosiglitazone	-1.49	0.0035	0.0096	700444	248674	annotated
1073	PC(2:0/0:0)	-1.03	0.0035	0.0097	849540	415455	annotated
4395	UDP	-1.42	0.0035	0.0098	175746	65485	annotated
1843	D-myo-Inositol 1,2-cyclic phosphate	-1.05	0.0037	0.0100	210864	101661	annotated
4924	SC-58125	-1.08	0.0036	0.0100	133290	62874	annotated
1606	3'-Amino-3'-deoxythymidine	-0.75	0.0037	0.0102	454549	269843	annotated
851	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	-1.14	0.0038	0.0104	1563746	708512	annotated
3820	Seriny-Threonine	-0.85	0.0040	0.0107	1149824	637617	annotated
3829	N-Acetyl-alpha-neuraminat	-0.62	0.0039	0.0107	1094999	713214	annotated
192	Leu-Gly-Pro	-2.07	0.0041	0.0111	349391	83488	annotated
1189	Histidinal	-1.28	0.0041	0.0111	905288	371548	annotated
1340	Cepharadione B	-1.01	0.0041	0.0111	671940	333929	annotated
5586	Chlorendic acid	0.75	0.0041	0.0111	15314	25817	annotated

2484	SM(d16:1/23:0)	0.56	0.0042	0.0114	60631	89440	annotated
902	Methionyl-Proline	-1.01	0.0043	0.0115	379276	187732	annotated
496	SM(d18:1/16:0)	0.46	0.0044	0.0116	7644809	10542473	annotated
2498	Fenpiclonil	-0.11	0.0043	0.0116	20131	18689	annotated
2930	2,2-Bis(4-hydroxyphenyl)hexafluoropropane	-0.55	0.0044	0.0116	15664955	10708768	annotated
4072	Valeric acid	-0.53	0.0043	0.0116	690383	477808	annotated
5047	Asparaginyln-Serine	-0.73	0.0045	0.0120	134687	80989	annotated
2119	cis-3-Hexenyl pyruvate	-0.97	0.0046	0.0122	206518	105459	annotated
460	Cysteinyl-Tyrosine	-0.88	0.0047	0.0124	84638	45833	annotated
624	2-Hydroxyadenine	-0.69	0.0047	0.0125	4093934	2530413	annotated
3015	Methyl benzoate	0.70	0.0049	0.0128	234908	380742	annotated
4358	1-Arachidonoylglycerophosphoinositol	-2.48	0.0049	0.0128	301277	54156	annotated
1050	2,6-Dibromohydroquinone	0.62	0.0049	0.0129	147365	225804	annotated
3258	Tetradecanedioic acid	-1.56	0.0050	0.0133	264814	89945	annotated
504	Buclizine	-1.18	0.0053	0.0138	4235612	1866665	annotated
4009	4-Hydroxycyclohexylcarboxylic acid	-0.58	0.0053	0.0139	908812	608785	annotated
105	N5-Acetyl-N2-gamma-L-glutamyl-L-ornithine	-1.01	0.0054	0.0140	99984	49638	annotated
4649	Stearoylglycerone phosphate	-0.86	0.0056	0.0144	168757	93269	annotated
122	Glutathione	-0.50	0.0056	0.0145	99544972	70541479	annotated+fragment
442	Isogingerenone B	1.16	0.0057	0.0147	5024876	11229959	annotated
222	L-2-Amino-3-(1-pyrazolyl)propanoic acid	-2.10	0.0057	0.0148	33726100	7870327	annotated
1870	N-Methylcalystegine B2	-0.31	0.0058	0.0149	427677	343791	annotated
1867	6-Acetylpicropolin	-0.55	0.0059	0.0151	388217	264822	annotated
4650	3R-hydroxy-decanoic acid	-0.65	0.0059	0.0151	156439	99670	annotated
441	L-Homocitrulline	1.66	0.0060	0.0152	678485	2139747	annotated
4057	UDP-D-Xylose	-1.00	0.0060	0.0154	313245	157136	annotated+fragment
1217	SM(d18:0/18:1(9Z))	0.52	0.0061	0.0155	740043	1062100	annotated
511	PE(24:1(15Z)/16:1(9Z))	-0.53	0.0061	0.0156	289578	200451	annotated
115	trans-4-Hydroxy-L-proline	-0.46	0.0064	0.0162	132304306	96146730	identified
106	Nicotianamine	-1.01	0.0065	0.0164	99984	49638	annotated

1538	FAD	-0.49	0.0065	0.0164	686690	489271	identified+fragment
5087	Deoxycoformycin	-0.71	0.0065	0.0164	86222	52680	annotated
2127	Linoleamide	-1.15	0.0066	0.0165	135745	61318	annotated
1436	Gamma-glutamyl-Gamma-glutamate	-0.69	0.0068	0.0171	332949	205850	annotated
1437	Gamma-glutamyl-Glutamine	-0.69	0.0068	0.0171	332949	205850	annotated
135	4-Guanidinobutanoate	-1.47	0.0069	0.0172	4852627	1748713	annotated+fragment
28	7-beta-D-Glucopyranosyloxybutylideneophthalide	-0.76	0.0069	0.0173	9156155	5394443	annotated
4172	3-Hydroxy-2-methyl-[S-(R,R)]-butanoic acid	-0.64	0.0070	0.0174	468685	300060	annotated
1402	PS(O-20:0/20:5(5Z,8Z,11Z,14Z,17Z))	-0.52	0.0070	0.0175	78584	54812	annotated
302	(x)-2-Heptanol glucoside	-4.22	0.0072	0.0179	46901	2511	annotated
4688	Tricozarin A	-4.52	0.0072	0.0179	184774	8077	annotated
2125	(E,E)-11,13-Octadecadien-9-ynoic acid	-0.96	0.0073	0.0180	113297	58203	annotated
2089	Glyburide	1.90	0.0074	0.0184	57278	214481	annotated
2396	Kanzonol V	-0.50	0.0075	0.0185	159198	112898	annotated
4925	2,3-Diphenyl-3-(2-pyridinyl)acrylonitrile	-1.43	0.0076	0.0187	85681	31848	annotated
1184	4E,15Z-Bilirubin IXa	-0.76	0.0077	0.0190	389426	229828	annotated
940	Epidermin	1.15	0.0078	0.0191	826922	1840480	annotated
1793	5-Methylcytidine	-0.93	0.0078	0.0191	272508	143329	annotated
2709	Hyperforin	0.55	0.0079	0.0193	19844	29024	annotated
131	5-Guanidino-2-oxopentanoate	-1.50	0.0081	0.0198	52161029	18483466	annotated
101	FMN	-0.66	0.0082	0.0200	194815	123217	identified
3994	PS(22:0/0:0)	-0.86	0.0083	0.0202	238563	131369	annotated
3236	Prorepensin	-3.33	0.0084	0.0204	96431	9568	annotated
1099	Histidinyl-Valine	-0.67	0.0085	0.0206	863072	541395	annotated
803	N6-(L-1,3-Dicarboxypropyl)-L-lysine	1.48	0.0086	0.0209	681845	1907988	annotated
1556	Domperidone	-1.04	0.0088	0.0212	613383	298299	annotated
1912	2-Methylpyrrole	-0.67	0.0092	0.0221	272477	171367	annotated
4256	DG(20:5n3/0:0/22:6n3)	3.12	0.0092	0.0221	30441	263788	annotated
1019	PA(20:1(11Z)/0:0)	-1.20	0.0093	0.0222	586791	255642	annotated
2310	PG(P-18:0/18:4(6Z,9Z,12Z,15Z))	-1.86	0.0094	0.0225	150516	41376	annotated

2756	PA(18:0/0:0)	-1.64	0.0094	0.0225	338643	108647	annotated
5101	Epoxyanethole	-0.79	0.0094	0.0225	101235	58512	annotated
1508	N-Formyl-L-methionine	0.74	0.0096	0.0230	298795	499119	annotated+fragment
1824	Hydroxypropyl-Threonine	0.75	0.0097	0.0232	192417	324550	annotated
1930	Oleoylcarnitine	-0.69	0.0098	0.0233	177016	109638	annotated
2263	N-Acetylputrescine	-0.87	0.0099	0.0236	143833	78801	annotated+fragment
1690	(2R,2'S)-Isobuteine	-1.85	0.0100	0.0238	476079	132243	annotated
4209	Thiosulfuric acid	-1.16	0.0101	0.0240	327208	146177	annotated
2138	Microlenin	-0.84	0.0103	0.0245	193472	107886	annotated
1734	alpha-Sinensal	0.87	0.0105	0.0248	209163	381947	annotated
1485	Glycylprolylhydroxyproline	-0.62	0.0106	0.0251	675448	438083	annotated
3213	Ethyl (±)-3-methylpentanoate	-0.48	0.0107	0.0251	10662020	7627100	annotated+fragment
3386	4-Methylnonanoic acid	-0.53	0.0109	0.0257	5044651	3498303	annotated+fragment
3002	Glycyl-Aspartate	-3.73	0.0111	0.0260	159532	12063	annotated
3975	Benzyl sulfate	-0.79	0.0111	0.0261	496288	287612	annotated
2201	Temurin	-1.33	0.0113	0.0265	130969	52069	annotated
4812	S-Allyl-L-cysteine	-1.05	0.0115	0.0268	154851	74539	annotated
3216	PS(20:3(8Z,11Z,14Z)/18:0)	0.43	0.0117	0.0273	1720402	2317054	annotated
5294	3,3'-Thiobispropanoic acid	-0.66	0.0118	0.0274	93719	59215	annotated
1435	Gamma-glutamyl-Serine	-0.66	0.0120	0.0279	656779	414839	annotated
5468	Norfluoxetine	-0.69	0.0120	0.0279	52412	32444	annotated
3885	UDP-glucuronate	1.27	0.0122	0.0282	197569	476905	annotated+fragment
4368	Phenylsulfate	-2.20	0.0124	0.0287	168764	36767	annotated
1169	Flavidulol C	-0.82	0.0127	0.0292	732271	414699	annotated
3714	Glyoxylate	-0.60	0.0127	0.0293	1561915	1030568	annotated
5325	Thiophanate-methyl	-0.64	0.0129	0.0296	86228	55289	annotated
4993	Procymidone	-0.70	0.0133	0.0307	50972	31311	annotated
1743	5S,6S-epoxy-15R-hydroxy-ETE	-1.24	0.0135	0.0310	375086	158268	annotated
4109	Imiquimod	-0.69	0.0137	0.0313	635577	394506	annotated
2379	Ethyl 2-benzylacetoacetate	-0.63	0.0137	0.0314	149602	96386	annotated

2094	N-Acetyldehydroanoinine	-0.59	0.0138	0.0316	211152	140623	annotated
3891	4-Oxononanal	-0.39	0.0143	0.0325	1075014	818106	annotated
4378	D-Arabinitol 1-phosphate	-0.82	0.0143	0.0325	212255	119964	annotated
353	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	-1.03	0.0144	0.0327	4119854	2018057	annotated
3455	Lauric acid	-0.52	0.0145	0.0328	3294058	2296147	annotated
535	Hexanoylglycine	-1.19	0.0146	0.0329	446074	195951	annotated
2249	2,4-Diamino-6-nitrotoluene	-1.05	0.0149	0.0335	100432	48460	annotated
1497	Mitiglinide	-1.26	0.0150	0.0337	123000	51340	annotated
454	N-Butyrylglycine	-0.65	0.0151	0.0340	6500110	4144461	annotated
2524	4'-Hydroxy-3'-prenylacetophenone	0.69	0.0156	0.0349	55613	89836	annotated
3712	(R)-2,3-Dihydroxypropane-1-sulfonate	-0.70	0.0155	0.0349	1400901	862209	annotated
2789	DCEBIO	0.53	0.0157	0.0350	1553663	2240626	annotated
1384	Phenylalanyl-Cysteine	1.33	0.0157	0.0351	285119	717475	annotated
5385	5,6-Dihydrouridine	-0.49	0.0158	0.0354	77383	55067	annotated
1648	Asparaginy-Valine	-0.75	0.0159	0.0355	294085	174661	annotated
2787	Ascorbate	0.55	0.0159	0.0355	50997476	74636746	annotated
2589	Valclavam	-3.42	0.0160	0.0356	57135	5333	annotated
4726	Hydroxypropyl-Asparagine	-0.63	0.0160	0.0356	177116	114190	annotated
4106	4-Deoxyerythronic acid	-0.60	0.0164	0.0363	508832	334595	annotated
1191	Alpha-CEHC	1.11	0.0165	0.0365	391390	845226	annotated
3445	4-[2,2-Dichloro-1-(4-methoxyphenyl)ethenyl]phenol	-1.66	0.0167	0.0368	26118	8289	annotated
3394	Brosimone I	-1.16	0.0170	0.0374	58975	26353	annotated
796	Lysyl-Alanine	-0.97	0.0174	0.0382	2143650	1096489	annotated
1226	PE(18:1(9Z)/15:0)	1.34	0.0176	0.0387	295174	748431	annotated
1224	Gamma-Glutamyl-Se-methylselenocysteine	-0.88	0.0177	0.0388	245495	133833	annotated
1955	hydroxyisovaleroyl carnitine	-0.60	0.0177	0.0388	259291	170851	annotated
1959	Daidzein 4'-O-glucuronide	-0.67	0.0177	0.0388	248305	155967	annotated
4792	gamma-L-Glutamyl-gamma-L-glutamyl-L-methionine	-1.36	0.0180	0.0395	59765	23207	annotated
1394	Glycyl-Arginine	-1.41	0.0183	0.0401	645279	242125	annotated
4258	2-Phosphinomethylmalate	-0.57	0.0188	0.0409	483476	326336	annotated

3696	(-)-Quebrachitol	-1.04	0.0190	0.0413	904514	440298	annotated
852	PC(20:3(8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z))	-0.77	0.0193	0.0417	2017769	1183312	annotated
5000	Phenylalanyl-Alanine	1.09	0.0194	0.0419	58019	123234	annotated
760	PE(20:1(11Z)/15:0)	-1.28	0.0198	0.0427	2341034	966540	annotated
2218	(R,S)-Nicotine	0.60	0.0198	0.0427	122435	185303	annotated
1855	Isobutyryl-L-carnitine	-1.05	0.0199	0.0429	160585	77301	annotated
4889	1-Cyano-2-hydroxy-3-butene	-0.64	0.0200	0.0431	136470	87834	annotated
433	S-(Hydroxyphenylacetothiohydroximoyl)-L-cysteine	-1.05	0.0201	0.0432	4192376	2024149	annotated
5358	2E,6E-Octadienal	-0.58	0.0205	0.0439	73198	48943	annotated
1456	Kiwiionoside	-0.85	0.0205	0.0440	658841	364384	annotated
4817	2,4,6-Triethyl-1,3,5-trioxane	-0.54	0.0206	0.0442	213882	146854	annotated
4862	Chondroitin	-0.67	0.0207	0.0443	107033	67046	annotated
1133	L-Albizziine	-1.18	0.0213	0.0454	1140730	502166	annotated
672	Lysyl-Valine	-1.54	0.0215	0.0457	3097109	1063468	annotated
925	Styrene	0.63	0.0219	0.0465	1595092	2461394	annotated
3736	Mollicellin C	-4.10	0.0221	0.0468	59436	3473	annotated
629	Histidinyl-Lysine	-1.16	0.0226	0.0477	110936	49692	annotated
685	N(pi)-Methyl-L-histidine	-0.77	0.0227	0.0479	4321985	2531172	identified+fragment
2307	3,5-Dimethoxytoluene	-0.50	0.0231	0.0488	173467	122692	annotated
1294	Dihydroferulic acid 4-sulfate	-0.43	0.0236	0.0497	297445	220073	annotated
4535	5-Hydroxymethyldeoxycytidylate	-0.67	0.0237	0.0498	88939	55893	annotated

CTL T0h vs CTL T24h

<i>Peak id</i>	<i>Metabolite</i>	<i>log fc</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T0h</i>	<i>Peak intensity CTL T24h</i>	<i>Identification</i>
505	Nonivamide	-2.21	0.000	0.000	3073320	666034	annotated
639	O-Propanoylcarnitine	2.83	0.000	0.000	865905	6168061	annotated
648	N-Formimino-L-glutamate	4.01	0.000	0.000	242114	3903789	annotated
713	N-a-Acetylcitrulline	-1.73	0.000	0.000	4325303	1307575	annotated
2196	(2S,2'S)-Pyrosaccharopine	1.59	0.000	0.000	40039	120395	annotated
3414	1-Deoxy-D-altro-heptulose 7-phosphate	-2.52	0.000	0.000	1966867	341830	annotated
3476	Monoethyl malonic acid	2.76	0.000	0.000	354413	2396789	annotated+fragment
221	Eplerenone	-3.32	0.000	0.000	26653823	2659892	annotated
503	alpha-Methylstyrene	-2.84	0.000	0.000	4415357	615323	annotated
712	PC(16:1(9Z)/0:0)	-1.30	0.000	0.000	4028181	1641273	annotated
1613	Rubraflavone D	1.60	0.000	0.000	242549	733739	annotated
2379	Ethyl 2-benzylacetoacetate	-1.30	0.000	0.000	149602	60839	annotated
4209	Thiosulfuric acid	-2.74	0.000	0.000	327208	49039	annotated
438	(3S)-3-Hydroxy-L-enduracididine	-2.11	0.000	0.000	9612745	2227891	annotated
4277	Nevirapine	0.95	0.000	0.000	278014	538561	annotated
4520	5'-xanthylate(2-)	1.50	0.000	0.000	141814	401289	annotated
1403	p-Hydroxyfelbamate	-2.09	0.000	0.000	837326	196823	annotated
318	N-Acetyl-beta-D-galactosamine	-1.38	0.000	0.001	3758856	1441752	annotated+fragment
146	beta-Alanine	-0.88	0.000	0.001	109481032	59616172	identified
317	N2-Acetyl-L-aminoadipate	-1.38	0.000	0.001	8229142	3160846	annotated
2003	Biotin	-5.22	0.000	0.001	199353	5348	annotated
2060	Octadecanedioic acid	0.97	0.000	0.001	67844	133344	annotated
5141	PG(21:0/17:2(9Z,12Z))	1.75	0.000	0.001	39691	133414	annotated
85	Dictyoquinazol B	-1.40	0.000	0.001	105806	39964	annotated
1508	N-Formyl-L-methionine	1.47	0.000	0.001	298795	827337	annotated+fragment

2836	D-Glucono-1,5-lactone	-1.25	0.000	0.001	1538292	645856	annotated
385	LysoPC(18:1(11Z))	-2.12	0.000	0.001	1459846	334696	annotated
3880	Dephospho-CoA	-2.07	0.000	0.001	575819	136901	annotated
504	Bucizine	-1.90	0.000	0.002	4235612	1136677	annotated
881	Isoleucyl-Leucine	-1.21	0.000	0.002	1979440	857611	annotated
3218	Citramalate	1.08	0.000	0.002	5207179	11022648	annotated+fragment
2962	N-Acetylgalactosamine 6-sulfate	-1.83	0.000	0.002	1717310	482391	annotated
3860	Pantetheine 4'-phosphate	-2.00	0.000	0.002	985738	247051	annotated
2374	Theasinensin C	-1.43	0.000	0.002	161242	59860	annotated
4367	N-Acetoxy-IQ	-1.01	0.000	0.003	396675	197462	annotated
2830	L-Aspartate	-1.06	0.000	0.003	73662101	35427470	identified
3379	Glycyl-Asparagine	-1.12	0.000	0.003	137641	63206	annotated
4191	3R-hydroxy-hexanoic acid	0.95	0.000	0.003	325636	629121	annotated
2120	3-Keto-scylo-inosamine	-1.16	0.000	0.003	267910	119624	annotated
4806	Sphingosine 1-phosphate	0.86	0.000	0.003	72546	131811	annotated
131	5-Guanidino-2-oxopentanoate	-2.40	0.000	0.003	52161029	9864748	annotated
3269	6,7-Benzocoumarin	-1.17	0.000	0.003	194509	86219	annotated
1549	L-4-Hydroxyglutamine	-1.05	0.000	0.003	796846	383700	annotated
1169	Flavidulol C	-1.32	0.000	0.004	732271	292808	annotated
1391	Methionyl-Leucine	-1.61	0.000	0.004	641475	210602	annotated
4236	L-phenylalanyl-L-hydroxyproline	-1.46	0.000	0.004	382678	139513	annotated
51	Homocarnosine	-1.01	0.000	0.005	6945894	3438762	annotated+fragment
1524	Dehydrocycloanthohumol hydrate	-1.75	0.000	0.005	527695	157385	annotated
285	LysoPC(20:3(5Z,8Z,11Z))	-1.70	0.000	0.005	480952	147934	annotated
1617	FPL64176	-1.57	0.000	0.006	495049	166935	annotated
5259	Lentialexin	0.83	0.000	0.006	62991	112068	annotated
2505	Normetanephrine	-0.65	0.000	0.006	106185	67453	annotated
205	L-Acetylcarnitine	1.10	0.000	0.007	24097812	51509609	annotated
1114	riboflavin	-1.12	0.000	0.008	1078849	495926	identified+fragment
456	Hydroxypropionylcarnitine	-1.49	0.000	0.008	974414	347692	annotated

4007	3-keto-n-caprylic acid	-0.77	0.000	0.008	977706	574498	annotated
2804	pyrophosphate	-2.73	0.000	0.009	9390607	1418222	identified
4535	5-Hydroxymethyldeoxycytidylate	-3.05	0.000	0.009	88939	10762	annotated
3522	N-Acetyl-alpha-D-galactosamine 1-phosphate	-1.30	0.000	0.009	1982767	806171	annotated
634	Didodecyl thiobispropanoate	1.11	0.000	0.009	1517503	3265728	annotated
640	2-Aminoheptanedioic acid	-2.36	0.000	0.009	3645320	712509	annotated
3553	PE(18:1(9Z)/0:0)	-1.13	0.000	0.010	2169480	992147	annotated
74	Gentianose	-1.62	0.000	0.010	269253	87591	annotated
3436	sn-Glycero-3-phospho-1-inositol	-1.02	0.000	0.010	4318326	2129772	annotated
2606	Homoveratric acid	1.26	0.001	0.010	23169	55351	annotated
2850	Aspartyl-Glutamine	-0.97	0.001	0.010	264417	135117	annotated
4262	Ipomeatetrahydrofuran	0.93	0.001	0.010	250796	479075	annotated
287	PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	-1.48	0.001	0.010	262580	93926	annotated
2484	SM(d16:1/23:0)	0.71	0.001	0.010	60631	98847	annotated
2789	DCEBIO	0.95	0.001	0.011	1553663	3002294	annotated
1745	13-Oxo-9,11-tridecadienoic acid	-0.81	0.001	0.011	490253	278901	annotated
919	SM(d18:1/23:0)	0.64	0.001	0.011	584604	910195	annotated
209	L-Tyrosine	-0.83	0.001	0.011	55242248	30981864	identified+fragment
220	Glycyl-Glutamine	-0.94	0.001	0.011	455091	237346	annotated
2964	Aspartyl-Serine	-1.00	0.001	0.011	1219080	611558	annotated
353	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	-1.55	0.001	0.012	4119854	1402328	annotated
2798	Clonidine	1.26	0.001	0.012	55516	132501	annotated
4954	Sulforaphane-N-acetylcysteine	-0.87	0.001	0.012	187428	102362	annotated
902	Methionyl-Proline	-1.45	0.001	0.012	379276	138921	annotated
1157	Histidinyl-Glutamine	-1.08	0.001	0.013	580078	275183	annotated
76	6-(alpha-D-Glucosaminy)-1D-myo-inositol	-1.68	0.001	0.013	237313	74086	annotated
832	Trimethylamine N-oxide	0.98	0.001	0.013	1217573	2394843	annotated
3850	Metsulfovax	0.66	0.001	0.013	960064	1518531	annotated
83	beta-D-Galactopyranosyl-(1->4)-2-amino-2-deoxy-beta-D-glucopyranosyl-(1->6)-D-mannose	-1.66	0.001	0.013	138242	43750	annotated

1560	Etorphine	-1.01	0.001	0.013	692509	344500	annotated
187	Pantothenic acid	-1.12	0.001	0.014	55220356	25463151	annotated+fragment
1691	Metronidazole	-1.37	0.001	0.014	498476	192852	annotated
2373	6-Keto-decanoylcarnitine	0.96	0.001	0.014	56771	110417	annotated
3198	Chloroform	0.38	0.001	0.014	12644282	16418887	annotated
751	Isolinderanolide	0.75	0.001	0.014	1641694	2769230	annotated
1065	(2R,3R)-3-Methylglutamyl-5-semialdehyde-N6-lysine	-1.54	0.001	0.015	220423	75714	annotated
609	Cohibin C	-0.51	0.001	0.016	4424735	3104654	annotated
629	HistidinyL-Lysine	-1.76	0.001	0.016	110936	32648	annotated
4898	2',3'-Cyclic UMP	-1.60	0.001	0.016	137330	45211	annotated
355	D-Glucosyldihydrosphingosine	4.48	0.001	0.017	47397	1054181	annotated
2010	3-Deoxyvitamin D3	-0.67	0.001	0.017	306827	192242	annotated
2787	Ascorbate	1.30	0.001	0.017	50997476	125727030	annotated
3411	Maleic acid	0.65	0.001	0.017	2685744	4216892	annotated+fragment
2878	Cycloprothrin	-1.00	0.001	0.018	174896	87682	annotated
3962	Hydroxycotinine	1.47	0.001	0.018	348042	963775	annotated
4039	3-Sulfinoalanine	-2.94	0.001	0.018	214199	27995	annotated
3108	Egonol	-1.25	0.001	0.018	131636	55429	annotated
3109	omega-Hydroxymoracin N	-1.25	0.001	0.018	131636	55429	annotated
61	Sakacin P	-0.93	0.001	0.020	1450810	763769	annotated
1365	PC(O-16:0/18:2(9Z,12Z))	0.53	0.002	0.020	700029	1010705	annotated
1710	3-Methylglutaryl carnitine	2.15	0.002	0.020	69365	308620	annotated
3363	3-(4-Hydroxyphenyl)pyruvate	-2.10	0.002	0.020	1267542	296183	annotated
1734	alpha-Sinensal	1.06	0.002	0.022	209163	436678	annotated
861	NADH	1.18	0.002	0.022	1001446	2273786	annotated
70	Polixetonium chloride	-1.59	0.002	0.023	718029	239267	annotated
455	Leucyl-Valine	-1.48	0.002	0.023	5832522	2084825	annotated
4692	Glucosamine 6-sulfate	-1.07	0.002	0.023	151223	72256	annotated
2182	Artemoin A	0.69	0.002	0.023	146297	235903	annotated
320	Gamma-glutamyl-Proline	-1.05	0.002	0.023	1549246	749982	annotated

1175	L-Coprine	-1.02	0.002	0.023	1129432	556795	annotated
3486	Phenylpropanoate	-1.81	0.002	0.023	1533153	436084	annotated
1327	PE-Cer(d14:1(4E)/22:0(2OH))	1.25	0.002	0.024	130045	309951	annotated
16	Hydroxypropyl-L-Valine	-0.69	0.002	0.024	1583226	982248	annotated
2215	Isocarbamid	-0.96	0.002	0.025	199179	102085	annotated
306	Sulforhodamine B	0.83	0.002	0.025	242480	429717	annotated
1491	Gamma-glutamyl-L-Phenylalanine	-1.32	0.002	0.025	217175	86933	annotated
1217	SM(d18:0/18:1(9Z))	0.62	0.002	0.026	740043	1140196	annotated
252	PC(18:0/0:0)	-0.58	0.002	0.027	46189582	30815666	annotated+fragment
175	Aspartyl-L-Proline	-0.96	0.002	0.027	764180	391720	annotated
784	Maleamate	-0.85	0.002	0.028	1963966	1090417	annotated
1550	Glycyl-L-Serine	-0.74	0.002	0.028	597863	358132	annotated
820	(Ac)2-L-Lys-D-Ala	-0.89	0.003	0.029	1111400	598876	annotated
2176	apo-[3-methylcrotonoyl-CoA:carbon-dioxide ligase (ADP-forming)]	0.95	0.003	0.029	94069	181811	annotated
3894	Methyl benzoate	0.68	0.003	0.029	617436	990387	annotated
216	Gamma-Glutamyltyrosine	-0.68	0.003	0.029	536367	335081	annotated
4726	Hydroxypropyl-L-Asparagine	-0.85	0.003	0.030	177116	97994	annotated
798	LysoPC(20:4(8Z,11Z,14Z,17Z))	-1.95	0.003	0.030	1872712	484761	annotated
1014	Isoleucyl-L-Threonine	-1.25	0.003	0.031	432163	181083	annotated
796	Lysyl-L-Alanine	-1.31	0.003	0.031	2143650	865940	annotated
4680	Asparaginyl-Gamma-glutamate	-0.83	0.003	0.031	77472	43621	annotated
5220	CDP-ribitol	0.70	0.003	0.031	66182	107445	annotated
2843	D-altro-D-manno-Heptose	-1.47	0.003	0.031	475563	172019	annotated
176	L-Tyrosine	-1.20	0.003	0.033	406807	177426	annotated
4400	Menthyl ethylene glycol carbonate	0.99	0.003	0.033	189068	375698	annotated
1656	2-Methylaminoadenosine	-1.01	0.003	0.033	334003	165375	annotated
423	Cysteineglutathione disulfide	-1.03	0.003	0.034	909965	446140	annotated
214	Hydroxypropyl-L-Serine	-0.82	0.003	0.034	1438368	813803	annotated
4134	5-Aminoimidazole	-0.64	0.003	0.034	752450	483361	annotated

3416	5-Oxoavermectin "2a" aglycone	-0.83	0.003	0.035	3330946	1872649	annotated+fragment
2119	cis-3-Hexenyl pyruvate	-1.05	0.003	0.035	206518	99619	annotated
4009	4-Hydroxycyclohexylcarboxylic acid	-0.59	0.004	0.036	908812	603875	annotated
605	PS(18:0/20:4(8Z,11Z,14Z,17Z))	0.66	0.004	0.036	3925743	6183434	annotated
628	Alanyl-Arginine	-2.01	0.004	0.037	2951357	735128	annotated
4934	Acetyl-CoA	-0.25	0.004	0.037	22118	18583	annotated
179	PE(22:1(13Z)/15:0)	-0.43	0.004	0.037	74578100	55416295	annotated
1150	1-O-Hexadecyl-lyso-sn-glycero-3-phosphocholine	0.64	0.004	0.037	903149	1405183	annotated
4903	1-Isothiocyanato-6-(methylthio)hexane	-0.96	0.004	0.037	150326	77138	annotated
3048	(S)C(S)S-S-Methylcysteine sulfoxide	0.77	0.004	0.038	1140696	1940506	annotated
262	cis-3-Hexenyl b-primeveroside	-2.05	0.004	0.038	132647	32119	annotated
1394	Glycyl-Arginine	-1.81	0.004	0.038	645279	183596	annotated
114	PE(22:2(13Z,16Z)/15:0)	0.82	0.004	0.038	89514594	158394884	annotated
218	Hydroxypropyl-Arginine	-1.02	0.004	0.038	468450	230308	annotated
3543	(all-E)-1,7-bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-one	-1.25	0.004	0.038	146992	61790	annotated
3509	Phenylacetic acid	0.79	0.004	0.039	1443888	2492751	annotated
1456	Kiwiionoside	-1.20	0.004	0.041	658841	286491	annotated
1466	Xestoaminol C	1.15	0.004	0.041	258090	570770	annotated
681	PE(20:0/14:1(9Z))	0.77	0.005	0.042	2636890	4488415	annotated
1404	N-Lignoceroylsphingosine	1.29	0.005	0.044	362893	890281	annotated
3712	(R)-2,3-Dihydroxypropane-1-sulfonate	-0.86	0.005	0.044	1400901	772376	annotated
66	Guanidinoacetate	-1.20	0.005	0.044	151638978	66078894	annotated+fragment
2924	L-alpha-glutamyl-L-hydroxyproline	-1.16	0.005	0.044	73054	32603	annotated
3096	Methylphosphate	-1.30	0.005	0.044	9014139	3666351	annotated
3196	Cer(d18:1/22:1(13Z))	-0.83	0.005	0.044	146166	82387	annotated
113	PE-NMe(18:1(9Z)/18:1(9Z))	0.35	0.005	0.045	125271366	160193220	annotated
5047	Asparaginyln-Serine	-0.76	0.005	0.045	134687	79614	annotated
361	Carnosine	-0.77	0.005	0.045	15285777	8939810	annotated+fragment
852	PC(20:3(8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z))	-0.91	0.005	0.045	2017769	1073874	annotated
14	Pterolactam	-0.42	0.005	0.045	682330064	510063752	annotated+fragment

3561	D-Biopterin	-0.84	0.005	0.045	141454	79246	annotated
1556	Domperidone	-1.19	0.005	0.045	613383	268239	annotated
3800	2-O-Benzoyl-D-glucose	-2.11	0.005	0.046	1008380	234203	annotated
1910	PC(P-18:1(11Z)/18:0)	0.51	0.005	0.046	273011	389671	annotated
740	Hydroxypropyl-Hydroxyproline	-0.73	0.005	0.047	3327208	2006531	annotated
755	PA(20:4(5Z,8Z,11Z,14Z)e/2:0)	1.68	0.006	0.048	105602	338200	annotated
411	L-Ornithine	-1.08	0.006	0.049	8423028	3979480	identified+fragment
1737	Lysyl-Threonine	-1.25	0.006	0.049	243597	102516	annotated
2744	ethyl tetradecanoate	-1.07	0.006	0.049	592208880	283032552	annotated

CTL T0h vs CTL T48h

<i>Peak id</i>	<i>Metabolite</i>	<i>log fc</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T0h</i>	<i>Peak intensity CTL T48h</i>	<i>Identification</i>
221	Eplerenone	-3.34	0.0000	0.0000	26653823	2628057	annotated
355	D-Glucosyldihydrospingosine	7.10	0.0000	0.0000	47397	6481706	annotated
504	Buclizine	-2.44	0.0000	0.0000	4235612	782779	annotated
505	Nonivamide	-2.01	0.0000	0.0000	3073320	760592	annotated
640	2-Aminoheptanedioic acid	-3.62	0.0000	0.0000	3645320	296804	annotated
2196	(2S,2'S)-Pyrosaccharopine	2.63	0.0000	0.0000	40039	247968	annotated
4148	1,4-beta-D-Glucan	-2.16	0.0000	0.0000	113919	25553	annotated
4806	Sphingosine 1-phosphate	1.21	0.0000	0.0000	72546	167943	annotated
4934	Acetyl-CoA	2.44	0.0000	0.0000	22118	119626	annotated
503	alpha-Methylstyrene	-2.91	0.0000	0.0001	4415357	588919	annotated
605	PS(18:0/20:4(8Z,11Z,14Z,17Z))	1.04	0.0000	0.0001	3925743	8084210	annotated
3216	PS(20:3(8Z,11Z,14Z)/18:0)	0.96	0.0000	0.0001	1720402	3345308	annotated
3476	Monoethyl malonic acid	1.67	0.0000	0.0001	354413	1128413	annotated+fragment
4050	SB 206553	-1.63	0.0000	0.0001	111390	36022	annotated
4520	5'-xanthylate(2-)	1.52	0.0000	0.0001	141814	407773	annotated
1006	Adenylsuccinic acid	2.52	0.0000	0.0002	315759	1809271	annotated+fragment
2964	Aspartyl-Serine	-1.48	0.0000	0.0002	1219080	438318	annotated
4516	9-Octadecenoic acid 1-[[[(1-oxohexadecyl)oxy]methyl]-2-(phosphonoxy)ethyl ester	1.02	0.0000	0.0003	214496	436227	annotated
832	Trimethylamine N-oxide	1.34	0.0000	0.0005	1217573	3086703	annotated
1216	5,6-Dihydroxyindole	-1.65	0.0000	0.0005	1018771	324507	annotated
187	Pantothenic acid	-1.47	0.0000	0.0009	55220356	19942956	annotated+fragment
3342	Ethylphosphate	-2.59	0.0000	0.0009	4251178	707467	annotated
3486	Phenylpropanoate	-2.38	0.0000	0.0009	1533153	295227	annotated
2830	L-Aspartate	-1.11	0.0000	0.0010	73662101	34116336	identified
4039	3-Sulfinioalanine	-2.20	0.0000	0.0010	214199	46688	annotated

303	AMP	1.27	0.0000	0.0011	12457422	30086573	identified+fragment
3885	UDP-glucuronate	2.17	0.0000	0.0011	197569	888109	annotated+fragment
306	Sulforhodamine B	1.15	0.0000	0.0012	242480	539261	annotated
961	dGDP	1.01	0.0000	0.0012	1042044	2100247	annotated+fragment
317	N2-Acetyl-L-aminoadipate	-1.23	0.0000	0.0013	8229142	3499476	annotated
318	N-Acetyl-beta-D-galactosamine	-1.24	0.0000	0.0013	3758856	1590161	annotated+fragment
2798	Clonidine	1.47	0.0000	0.0013	55516	153871	annotated
2789	DCEBIO	1.18	0.0000	0.0014	1553663	3512866	annotated
1743	5S,6S-epoxy-15R-hydroxy-ETE	-2.16	0.0001	0.0015	375086	84210	annotated
1745	13-Oxo-9,11-tridecadienoic acid	-0.97	0.0001	0.0015	490253	250565	annotated
2040	Triethylene Glycol Monomethyl Ether	-1.84	0.0001	0.0018	212641	59201	annotated
3046	Potassium 2-(1'-ethoxy) ethoxypropanoate	-2.47	0.0001	0.0018	5250992	946603	annotated
3213	Ethyl (±)-3-methylpentanoate	-0.76	0.0001	0.0018	10662020	6280567	annotated+fragment
1990	5-Aminopentanamide	1.33	0.0001	0.0019	110554	277500	annotated
2797	1-(Isothiocyanatomethyl)-4-methoxybenzene	1.65	0.0001	0.0020	52367	164019	annotated
3015	Methyl benzoate	1.04	0.0001	0.0020	234908	481414	annotated
66	Guanidinoacetate	-1.84	0.0001	0.0021	151638978	42464317	annotated+fragment
2459	N-Isovaleryl-L-homoserine lactone	-0.86	0.0001	0.0021	127097	69783	annotated
3108	Egonol	-1.53	0.0001	0.0021	131636	45466	annotated
3109	omega-Hydroxymoracin N	-1.53	0.0001	0.0021	131636	45466	annotated
2215	Isocarbamid	-1.28	0.0001	0.0022	199179	81903	annotated
1549	L-4-Hydroxyglutamine	-1.07	0.0001	0.0024	796846	379968	annotated
1856	N4-(Acetyl-beta-D-glucosaminy)asparagine	0.93	0.0001	0.0025	190877	364632	annotated
4364	Coenzyme A	2.21	0.0001	0.0027	82468	381352	annotated
4007	3-keto-n-caprylic acid	-0.81	0.0001	0.0028	977706	557747	annotated
85	Dictyoquinazol B	-2.55	0.0001	0.0029	105806	18017	annotated
1311	2,3-Butanediol glucoside	2.43	0.0002	0.0035	58975	317421	annotated
3344	3-Deoxy-D-manno-octulosonate 8-phosphate	-3.15	0.0002	0.0037	140556	15889	annotated
79	cis-N-Methyl-(S)-7,8,13,14-tetrahydroprotoberberine	-1.79	0.0002	0.0038	216235	62562	annotated
2787	Ascorbate	1.78	0.0002	0.0038	50997476	174863272	annotated

3979	Fucose 1-phosphate	2.20	0.0002	0.0042	200931	923545	annotated
3012	Isosyringinoside	2.04	0.0002	0.0043	425437	1753402	annotated
639	O-Propanoylcarnitine	1.58	0.0002	0.0048	865905	2596480	annotated
2927	Asparaginyl-Proline	-1.43	0.0003	0.0051	48330	17996	annotated
2327	CL(1'-[18:2(9Z,12Z)/0:0],3'-[18:2(9Z,12Z)/0:0])	-1.74	0.0003	0.0054	92293	27704	annotated
2843	D-altro-D-manno-Heptose	-2.17	0.0003	0.0058	475563	105752	annotated
3257	Phenylpropionylglycine	-1.51	0.0003	0.0058	885904	310173	annotated
4688	Tricozarin A	-2.85	0.0003	0.0058	184774	25702	annotated
617	Fenugreekine	1.26	0.0003	0.0065	3213564	7672746	annotated+fragment
416	(S)-Codamine	-1.61	0.0004	0.0067	83982	27533	annotated
3028	N6-Carbamoyl-L-threonyladenosine	1.00	0.0004	0.0067	27029	53954	annotated
3894	Methyl benzoate	0.84	0.0004	0.0070	617436	1105777	annotated
2250	Myricetin 3,3'-digalactoside	2.77	0.0004	0.0075	22054	150394	annotated
2374	Theasinensin C	-1.30	0.0004	0.0075	161242	65261	annotated
2850	Aspartyl-Glutamine	-0.97	0.0004	0.0075	264417	134693	annotated
715	Valerylglycine	0.91	0.0004	0.0077	2521886	4726180	annotated
2086	2-Hydroxy-3-methyl-9H-carbazole	-0.93	0.0005	0.0078	30103	15789	annotated
3839	Uridine diphosphate glucose	3.66	0.0005	0.0078	68975	872739	annotated+fragment
3704	Myristicin	-1.21	0.0005	0.0082	20472	8876	annotated
4256	DG(20:5n3/0:0/22:6n3)	3.67	0.0005	0.0084	30441	386916	annotated
3014	N-Succinyl-2-L-amino-6-oxoheptanedioate	1.03	0.0006	0.0092	277813	568419	annotated
3211	PS(18:0/18:1(9Z))	0.58	0.0006	0.0093	1504004	2244309	annotated
46	Adenosine	1.13	0.0006	0.0100	113782140	249397612	identified+fragment
4825	GDP-3,6-dideoxy-D-galactose	1.96	0.0007	0.0103	29770	116102	annotated
3543	(all-E)-1,7-bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-one	-1.57	0.0007	0.0104	146992	49526	annotated
861	NADH	1.25	0.0007	0.0113	1001446	2382872	annotated
3209	2-Hydroxy-2-(2-oxopropyl)butanedioic acid	0.98	0.0008	0.0118	5524580	10863228	annotated
411	L-Ornithine	-1.38	0.0008	0.0120	8423028	3242198	identified+fragment
2292	Gabapentin	-0.65	0.0008	0.0120	202723	129256	annotated
3212	PI(18:0/16:0)	0.67	0.0008	0.0120	858051	1366342	annotated

302	(x)-2-Heptanol glucoside	-3.21	0.0009	0.0123	46901	5061	annotated
2119	cis-3-Hexenyl pyruvate	-1.16	0.0009	0.0123	206518	92691	annotated
3379	Glycyl-Asparagine	-1.03	0.0008	0.0123	137641	67521	annotated
3194	Cer(d18:0/16:0)	-1.02	0.0009	0.0125	810230	400091	annotated
3833	N-Acetyl-L-methionine	-1.17	0.0009	0.0125	632629	281115	annotated
4686	Maltopentaose	-1.86	0.0010	0.0137	174884	48223	annotated
1818	Dimorphecolic acid	-0.85	0.0010	0.0140	376440	209469	annotated
13	Prolyl-Valine	-1.26	0.0011	0.0147	1047546	437171	annotated
2606	Homoveratric acid	1.07	0.0011	0.0147	23169	48807	annotated
740	Hydroxypropyl-Hydroxyproline	-0.84	0.0011	0.0151	3327208	1853158	annotated
47	Dichotosinin	0.96	0.0012	0.0154	1604506	3131090	annotated
4862	Chondroitin	0.92	0.0013	0.0166	107033	202899	annotated
74	Gentianose	-1.55	0.0013	0.0170	269253	91715	annotated
1780	L-Cystine	-1.65	0.0013	0.0170	301284	95803	identified
5220	CDP-ribitol	0.72	0.0013	0.0171	66182	109314	annotated
3725	Dambonitol	-2.31	0.0014	0.0182	974900	197128	annotated
820	(Ac)2-L-Lys-D-Ala	-0.94	0.0015	0.0187	1111400	579854	annotated
4236	L-phenylalanyl-L-hydroxyproline	-1.56	0.0016	0.0193	382678	129999	annotated
611	PG(18:1(9Z)/18:1(11Z))	0.56	0.0017	0.0200	962945	1420934	annotated
3509	Phenylacetic acid	0.91	0.0016	0.0200	1443888	2720910	annotated
3522	N-Acetyl-alpha-D-galactosamine 1-phosphate	-1.10	0.0018	0.0209	1982767	922941	annotated
273	Mefenacet	-1.10	0.0019	0.0218	211969	98611	annotated
3411	Maleic acid	0.64	0.0020	0.0225	2685744	4188140	annotated+fragment
4277	Nevirapine	0.60	0.0020	0.0227	278014	421745	annotated
1217	SM(d18:0/18:1(9Z))	0.61	0.0021	0.0234	740043	1127210	annotated
83	beta-D-Galactopyranosyl-(1->4)-2-amino-2-deoxy-beta-D-glucopyranosyl-(1->6)-D-mannose	-1.53	0.0022	0.0239	138242	47827	annotated
2966	D-Glycero-D-galacto-heptitol	-4.33	0.0022	0.0239	370598	18384	annotated
4856	Apigenin 7-sulfate	-1.22	0.0022	0.0240	117649	50630	annotated
180	PC(20:2(11Z,14Z)/16:1(9Z))	0.42	0.0023	0.0245	31352215	42038592	annotated

3261	butylisobutyrate (+ isobutylisobutyrate)	-0.62	0.0023	0.0246	8462694	5504265	annotated+fragment
1307	11-amino-undecanoic acid	-1.28	0.0025	0.0262	338756	139943	annotated
1734	alpha-Sinensal	1.10	0.0025	0.0264	209163	447173	annotated
1910	PC(P-18:1(11Z)/18:0)	0.54	0.0025	0.0265	273011	396572	annotated
454	N-Butyrylglycine	0.70	0.0026	0.0271	6500110	10526485	annotated
76	6-(alpha-D-Glucosaminy)-1D-myo-inositol	-1.59	0.0027	0.0281	237313	78625	annotated
4470	Myricetin 3-arabinoside	1.86	0.0028	0.0283	95550	346978	annotated
758	PG(18:3(6Z,9Z,12Z)/18:1(9Z))	-0.82	0.0028	0.0284	190681	107966	annotated
1489	Arginyl-Proline	-1.14	0.0029	0.0290	559077	253805	annotated
972	Butabarbital	-1.55	0.0029	0.0291	1228082	418956	annotated
5172	8-Oxo-dGDP	0.82	0.0029	0.0291	64968	114620	annotated
608	PS(18:0/18:0)	0.45	0.0029	0.0293	4886051	6676606	annotated
4680	Asparaginy-Gamma-glutamate	-0.87	0.0030	0.0299	77472	42358	annotated
1585	16alpha-Bromo-17beta-estradiol	2.34	0.0031	0.0301	116812	592318	annotated
338	Tromethamine	1.93	0.0031	0.0303	1564722	5942815	annotated+fragment
2307	3,5-Dimethoxytoluene	-0.66	0.0031	0.0304	173467	110026	annotated
3045	Uracil	-0.90	0.0032	0.0307	14769556	7923718	annotated
2379	Ethyl 2-benzylacetoacetate	-0.77	0.0032	0.0313	149602	87880	annotated
1550	Glycyl-Serine	-0.71	0.0033	0.0315	597863	366318	annotated
1524	Dehydrocycloanthohumol hydrate	-1.94	0.0034	0.0327	527695	137856	annotated
974	PC(O-20:0/12:0)	0.65	0.0035	0.0330	1290362	2024411	annotated
49	Tolbutamide	0.95	0.0035	0.0332	114238	220792	annotated
3975	Benzyl sulfate	1.04	0.0036	0.0334	496288	1023463	annotated
209	L-Tyrosine	-0.72	0.0037	0.0346	55242248	33484049	identified+fragment
2913	Alloxanthine	-0.88	0.0038	0.0347	48985366	26534368	annotated+fragment
207	NG,NG-Dimethyl-L-arginine	-1.59	0.0039	0.0356	38060983	12654624	annotated
1384	Phenylalanyl-Cysteine	1.55	0.0041	0.0365	285119	836968	annotated
2999	hexyl propionate	-0.51	0.0041	0.0365	31442355	22031321	annotated
3179	Xanthosine	-1.33	0.0041	0.0369	1258177	500395	annotated+fragment
341	Dulxanthone E	0.70	0.0043	0.0379	12410398	20155139	annotated+fragment

1584	PE(18:3(6Z,9Z,12Z)/0:0)	0.89	0.0046	0.0394	392066	726194	annotated
607	Glycidyl oleate	0.48	0.0046	0.0395	5807191	8073406	annotated
788	Histidiny-Glycine	-0.64	0.0046	0.0395	3160522	2032175	annotated
3004	Brugine	-1.15	0.0046	0.0395	11011	4965	annotated
3072	Threonolactone	1.03	0.0046	0.0395	10088155	20633708	annotated+fragment
3372	Mannitol	-1.62	0.0049	0.0414	2808482	911794	annotated
1365	PC(O-16:0/18:2(9Z,12Z))	0.46	0.0049	0.0418	700029	964665	annotated
2930	2,2-Bis(4-hydroxyphenyl)hexafluoropropane	-0.54	0.0050	0.0419	15664955	10774077	annotated
3468	PS(18:0/22:5(7Z,10Z,13Z,16Z,19Z))	0.84	0.0050	0.0422	2009449	3604764	annotated
59	L-Alloisoleucine	-0.71	0.0051	0.0425	201673344	123204500	annotated+fragment
2838	CMP	-1.28	0.0051	0.0428	1093147	448889	identified+fragment
1849	Seriny-Tyrosine	1.17	0.0052	0.0431	155935	351309	annotated
2744	ethyl tetradecanoate	-1.07	0.0056	0.0456	592208880	282127268	annotated
4057	UDP-D-Xylose	1.04	0.0057	0.0459	313245	643275	annotated+fragment
137	L-Methionine	-0.82	0.0057	0.0461	88358132	49906705	identified+fragment
876	Carboxy-ibuprofen	0.90	0.0059	0.0469	949306	1767438	annotated
877	2,3-Dehydrosalvipisone	0.78	0.0060	0.0478	253220	434249	annotated
1617	FPL64176	-1.08	0.0062	0.0489	495049	234235	annotated
634	Didodecyl thiobispropanoate	0.88	0.0063	0.0496	1517503	2801635	annotated
3032	Norambreinolide	-1.17	0.0064	0.0500	616103	273107	annotated

Dietary effect- LPS effect- metabolomics pilot study on liver samples (identified and annotated metabolites)

CTL T0h vs CTS T0h

<i>Peak id</i>	<i>Metabolite</i>	<i>Log FC</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T0h</i>	<i>Peak intensity CTS T0h</i>	<i>Identification</i>
355	D-Glucosyldihydrosphingosine	//	0.0000	0.0000	47397	0	annotated
2060	Octadecanedioic acid	2.01	0.0000	0.0001	67844	273756	annotated
2046	2-Octenoylcarnitine	//	0.0000	0.0005	0	19569	annotated
133	L-Citrulline	1.41	0.0000	0.0052	15024106	39994451	identified+fragment
221	Eplerenone	-2.76	0.0000	0.0052	26653823	3923876	annotated
505	Nonivamide	-1.60	0.0000	0.0052	3073320	1015122	annotated
1631	Captopril	1.29	0.0001	0.0061	261605	638140	annotated
4914	Methyl methanesulfonate	2.58	0.0001	0.0091	19447	116412	annotated
503	alpha-Methylstyrene	-2.32	0.0001	0.0095	4415357	885866	annotated
2866	Phenol	0.69	0.0002	0.0172	28376953	45830406	annotated
391	PC(20:2(11Z,14Z)/14:1(9Z))	0.77	0.0003	0.0251	6549220	11184740	annotated
163	L-Pipecolate	1.27	0.0004	0.0281	13576822	32712583	annotated
2606	Homoveratric acid	1.22	0.0004	0.0293	23169	54140	annotated
1367	L-glycyl-L-hydroxyproline	0.88	0.0004	0.0312	532438	980030	annotated
2597	1-(1-Pyrrolidinyl)-2-propanone	0.60	0.0004	0.0312	53670	81141	annotated
5267	Pemirolast	-0.88	0.0005	0.0320	98971	53714	annotated

3833	N-Acetyl-L-methionine	1.13	0.0005	0.0337	632629	1382115	annotated
2292	Gabapentin	-0.67	0.0005	0.0366	202723	127439	annotated
499	Difloxacin	1.51	0.0006	0.0391	125859	358954	annotated
4044	D-Erythrose 4-phosphate	1.37	0.0006	0.0391	255973	660035	annotated
5243	1D-myo-Inositol 1,4-bisphosphate	1.38	0.0007	0.0397	36605	95129	annotated
504	Buclizine	-1.54	0.0007	0.0406	4235612	1456387	annotated
3047	Homocysteinesulfinic acid	0.78	0.0008	0.0469	1699994	2917702	annotated
4464	Epoxiconazole	-1.43	0.0009	0.0500	59835	22181	annotated

CTL T12h vs CTS T12h

<i>Peak id</i>	<i>Metabolite</i>	<i>log FC</i>	<i>p</i>	<i>Adjusted p</i>	<i>Peak intensity CTL T12h</i>	<i>Peak intensity CTS T12h</i>	<i>Identification</i>
1	Betaine	0.97	0.000	0.0000	136620676	267057100	identified+fragment
11	2-Acetylpyrazine	1.32	0.000	0.0000	619267838	154809827	annotated+fragmen
12	L-isoleucyl-L-proline	-5.66	0.000	0.0000	208314568	4117926	annotated
13	Prolyl-Valine	1.42	0.000	0.0000	396784	1059782	annotated
14	Pterolactam	1.79	0.000	0.0000	235015200	814387232	annotated+fragmen
15	Dulxanthone F	-3.38	0.000	0.0000	97534800	9399925	annotated+fragmen
16	Hydroxypropyl-Valine	0.23	0.000	0.0000	1563617	1833851	annotated
23	Neurine	2.70	0.000	0.0000	91825451	597654984	annotated
27	Choline phosphate	1.15	0.000	0.0000	198816456	442474952	identified
28	7-beta-D-Glucopyranosyloxybutylidenephthalide	-2.16	0.000	0.0000	57962193	12953153	annotated
31	Hypoxanthine	2.52	0.000	0.0000	56656878	326040096	identified+fragment
33	Pyridine N-oxide glucuronide	-2.68	0.000	0.0000	17355895	2703026	annotated
35	5-Hydroxytryptophan	1.49	0.000	0.0000	159091	445710	annotated
59	L-Alloisoleucine	2.48	0.000	0.0000	46987332	261786704	annotated+fragmen
60	L-Kynurenine	-1.62	0.000	0.0000	17241694	5625174	identified+fragment
61	Sakacin P	1.23	0.000	0.0000	614482	1439035	annotated
62	5-Hydroxyindoleacetate	2.14	0.000	0.0000	362653	1603006	annotated
66	Guanidinoacetate	3.69	0.000	0.0000	17897304	230527888	annotated+fragmen
70	Polixetonium chloride	-3.69	0.000	0.0000	7879967	610138	annotated
74	Gentianose	2.29	0.000	0.0000	43395	211683	annotated
76	6-(alpha-D-Glucosaminy)-1D-myo-inositol	2.77	0.000	0.0000	29327	200654	annotated
77	Lactosamine	2.78	0.000	0.0000	28002	192092	annotated
79	cis-N-Methyl-(S)-7,8,13,14-tetrahydroprotoberberine	3.22	0.000	0.0000	31893	297148	annotated

83	beta-D-Galactopyranosyl-(1->4)-2-amino-2-deoxy-beta-	2.40	0.000	0.0000	24072	127302	annotated
85	Dictyoquinazol B	4.99	0.000	0.0000	4621	146794	annotated
91	2S-amino-butanoic acid	1.05	0.000	0.0000	57994412	120408506	annotated+fragmen
94	Methyl N-methylantranilate	1.81	0.000	0.0000	52845325	185183152	annotated+fragmen
95	L-gamma-glutamyl-L-leucine	-1.45	0.000	0.0000	9973351	3652994	annotated
96	Glutamylphenylalanine	1.56	0.000	0.0000	729106	2143947	annotated
97	Phensuximide	1.68	0.000	0.0000	275569	881297	annotated
99	Coformycin	1.89	0.000	0.0000	119233	443362	annotated
101	FMN	1.41	0.000	0.0000	119897	318297	identified
105	N5-Acetyl-N2-gamma-L-glutamyl-L-ornithine	1.58	0.000	0.0000	61834	185024	annotated
106	Nicotianamine	1.90	0.000	0.0000	49638	185024	annotated
116	L-Valine	1.62	0.000	0.0000	50048747	153379136	identified+fragment
117	N-Alpha-acetyllysine	0.58	0.000	0.0000	13260348	19867597	annotated+fragmen
119	Sesamolin	2.01	0.000	0.0000	1126044	4522258	annotated
128	L-Glutamate	1.27	0.000	0.0000	61795585	148549786	identified+fragment
129	Hydroxypropyl-Proline	-2.85	0.000	0.0000	21189795	2948746	annotated
131	5-Guanidino-2-oxopentanoate	3.51	0.000	0.0000	12070848	137945250	annotated
133	L-Citrulline	2.62	0.000	0.0000	15388150	94526498	identified+fragment
137	L-Methionine	2.64	0.000	0.0000	18339888	114298440	identified+fragment
139	Isoleucyl-Aspartate	-2.14	0.000	0.0000	6095521	1380044	annotated+fragmen
140	Tos-Arg-CH2Cl	2.43	0.000	0.0000	229211	1236328	annotated
146	beta-Alanine	1.82	0.000	0.0000	26959159	94882372	identified
149	L-Arginine	1.48	0.000	0.0000	37983687	105946074	identified+fragment
161	PC(16:0/0:0)	1.28	0.000	0.0000	46418562	112792838	annotated
162	PC(18:3(6Z,9Z,12Z)/0:0)	-3.30	0.000	0.0000	13806606	1397812	annotated
163	L-Pipecolate	4.45	0.000	0.0000	4460809	97783146	annotated
168	Nicotinamide	1.66	0.000	0.0000	29173622	92235718	identified+fragment
170	L-homoserine	1.94	0.000	0.0000	24503412	94174260	identified+fragment

171	(5-L-Glutamyl)-L-glutamine	-1.23	0.000	0.0000	10456454	4462687	annotated
173	Alanyl-Aspartate	1.58	0.000	0.0000	480905	1440011	annotated
175	Aspartyl-Proline	1.90	0.000	0.0000	221745	826147	annotated
176	L-Tyrosine	1.80	0.000	0.0000	142206	494242	annotated
180	PC(20:2(11Z,14Z)/16:1(9Z))	0.34	0.000	0.0000	34338776	43515706	annotated
187	Pantothenic acid	2.82	0.000	0.0000	9210027	64964342	annotated+fragmen
188	S-Acetyldihydrolipoamide	1.83	0.000	0.0000	19964181	70736231	annotated
199	3-Acetylthiophene	1.96	0.000	0.0000	135712	526357	annotated
202	N-Butyryl-L-homoserine lactone	1.66	0.000	0.0000	110685	348825	annotated
205	L-Acetylcarnitine	1.78	0.000	0.0000	21172347	72826432	annotated
207	NG,NG-Dimethyl-L-arginine	3.09	0.000	0.0000	8529546	72397903	annotated
209	L-Tyrosine	2.33	0.000	0.0000	13316641	66731657	identified+fragment
214	Hydroxypropyl-Serine	-1.92	0.000	0.0000	4321748	1145963	annotated
216	Gamma-Glutamyltyrosine	1.11	0.000	0.0000	243737	524960	annotated
224	3beta,6beta-Dihydroxynortropane	1.43	0.000	0.0000	19691069	53179717	annotated
225	L-Lysine	2.05	0.000	0.0000	16418266	67950599	identified+fragment
230	Nalbuphine	-2.18	0.000	0.0000	4454880	980891	annotated
266	L-Serine	2.52	0.000	0.0000	7370024	42195865	identified+fragment
270	Glycyl-Lysine	-2.41	0.000	0.0000	3343869	627845	annotated
273	Mefenacet	2.55	0.000	0.0000	52145	305916	annotated
277	Adenine	1.33	0.000	0.0000	16202056	40709146	identified+fragment
278	PC(18:2(9Z,12Z)/0:0)	1.43	0.000	0.0000	13082162	35342161	annotated
281	Ergothioneine	1.20	0.000	0.0000	12009651	27496471	annotated
282	Tetrahydropentoxyline	-0.76	0.000	0.0000	4025195	2378461	annotated
291	PC(15:0/0:0)	1.89	0.000	0.0000	6266816	23207092	annotated
292	PE(20:4(5Z,8Z,11Z,14Z)/0:0)	0.29	0.000	0.0000	3078273	3772945	annotated
296	Allopurinol riboside	1.27	0.000	0.0000	11229986	27001567	annotated+fragmen
303	AMP	-1.09	0.000	0.0000	13999092	6588582	identified+fragment

306	Sulforhodamine B	-5.14	0.000	0.0000	3784956	107144	annotated
316	Indoleacrylic acid	2.08	0.000	0.0000	5432815	23009065	annotated
317	N2-Acetyl-L-aminoadipate	2.02	0.000	0.0000	2226019	9000066	annotated
318	N-Acetyl-beta-D-galactosamine	1.92	0.000	0.0000	1051508	3969177	annotated+fragmen
319	Histidinyl-Serine	1.50	0.000	0.0000	1000392	2824295	annotated+fragmen
320	Gamma-glutamyl-Proline	1.46	0.000	0.0000	548592	1508266	annotated
326	Piperidine	1.68	0.000	0.0000	6226553	20007172	annotated+fragmen
329	N2,N2-Dimethylguanosine	-1.88	0.000	0.0000	1756740	478358	annotated
337	1-(beta-D-Ribofuranosyl)-1,4-dihyronicotinamide	3.15	0.000	0.0000	1249797	11062795	annotated
353	(S)-2,3,4,5-Tetrahydropyridine-2-carboxylate	3.23	0.000	0.0000	1572625	14731259	annotated
375	Thiomorpholine 3-carboxylate	2.20	0.000	0.0000	2613644	12021418	annotated
385	LysoPC(18:1(11Z))	0.86	0.000	0.0000	810245	1465675	annotated
411	L-Ornithine	2.48	0.000	0.0000	2133712	11908962	identified+fragment
416	(S)-Codamine	-1.58	0.000	0.0000	374041	125267	annotated
422	(5-L-Glutamyl)-L-glutamate	5.04	0.000	0.0000	345005	11351411	annotated+fragmen
423	Cysteineglutathione disulfide	2.15	0.000	0.0000	403528	1797043	annotated
424	N6-Methyladenosine	2.36	0.000	0.0000	154958	794240	annotated
426	N6,N6,N6-Trimethyl-L-lysine	2.64	0.000	0.0000	1956985	12175422	annotated+fragmen
435	Orthophosphate	1.21	0.000	0.0000	5382501	12444314	annotated
443	S-Prenyl-L-cysteine	1.29	0.000	0.0000	3967605	9699224	annotated
448	Creatinine	1.42	0.000	0.0000	4555200	12222408	identified+fragment
456	Hydroxypropionylcarnitine	0.58	0.000	0.0000	1552635	2328779	annotated
460	Cysteiny-Tyrosine	-0.47	0.000	0.0000	262543	190078	annotated
471	5,6-Dihydroxyprostaglandin F1a	3.97	0.000	0.0000	16370	256773	annotated
474	2,3-Dihydro-2,3-dihydroxy-4-(4-methoxyphenyl)-1H-	1.90	0.000	0.0000	32107	119890	annotated
475	Hexahydro-2',4-dimethylspiro[1,3-dithiolo[4,5-c]furan-	4.39	0.000	0.0000	5059	106036	annotated
481	Choline sulfate	1.81	0.000	0.0000	2797898	9836615	annotated
499	Difloxacin	-2.04	0.000	0.0000	2694298	654187	annotated

513	5-Hydroxymethyl-4-methyluracil	2.16	0.000	0.0000	1373737	6152915	annotated+fragmen
517	Hypotaurine	1.44	0.000	0.0000	3449430	9344990	annotated
534	1H-Imidazole-1-acetic acid	1.91	0.000	0.0000	1930969	7279212	annotated+fragmen
535	Hexanoylglycine	1.50	0.000	0.0000	375450	1065584	annotated
612	PG(P-16:0/20:3(8Z,11Z,14Z))	0.12	0.000	0.0000	193041	210142	annotated
634	Didodecyl thiobispropanoate	-1.47	0.000	0.0000	3562935	1285998	annotated
640	2-Aminoheptanedioic acid	2.61	0.000	0.0000	444358	2706489	annotated
693	Cytidine	1.77	0.000	0.0000	1622648	5543777	identified
704	N-gamma-L-Glutamyl-L-methionine	1.76	0.000	0.0000	439755	1492696	annotated
707	3'-O-Methylguanosine	2.20	0.000	0.0000	162670	747453	annotated+fragmen
712	PC(16:1(9Z)/0:0)	1.36	0.000	0.0000	1226059	3146456	annotated
713	N-a-Acetylcitrulline	1.98	0.000	0.0000	845721	3343919	annotated
721	Phosphonoacetaldehyde	0.74	0.000	0.0000	3239401	5417168	annotated
740	Hydroxypropyl-Hydroxyproline	1.22	0.000	0.0000	1294582	3020744	annotated
746	Alanyl-Proline	1.19	0.000	0.0000	1636013	3742001	annotated
751	Isolinderanolide	1.31	0.000	0.0000	1592891	3962389	annotated
752	1-(11Z,14Z-eicosadienoyl)-glycero-3-phosphate	2.03	0.000	0.0000	726455	2965137	annotated
757	sn-3-O-(geranylgeranyl)glycerol 1-phosphate	1.91	0.000	0.0000	131905	496880	annotated
758	PG(18:3(6Z,9Z,12Z)/18:1(9Z))	1.32	0.000	0.0000	171742	428626	annotated
767	Midodrine	1.47	0.000	0.0000	766133	2115637	annotated
784	Maleamate	2.03	0.000	0.0000	535161	2192952	annotated
787	2,3-dihydroxy-valeric acid	0.22	0.000	0.0000	226111	264084	annotated
791	Oxidized glutathione	2.17	0.000	0.0000	726367	3278188	annotated+fragmen
804	Ne,Ne dimethyllysine	2.68	0.000	0.0000	453803	2914700	annotated
820	(Ac)2-L-Lys-D-Ala	1.21	0.000	0.0000	421495	977911	annotated
851	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	1.26	0.000	0.0000	962839	2306642	annotated
868	L-Histidine trimethylbetaine	1.51	0.000	0.0000	789682	2248798	annotated
876	Carboxy-ibuprofen	-1.57	0.000	0.0000	2606473	880344	annotated

881	Isoleucyl-Leucine	1.65	0.000	0.0000	668706	2096243	annotated
896	Phosphodimethylethanolamine	1.61	0.000	0.0000	575598	1760171	annotated
914	Purine	2.26	0.000	0.0000	223962	1076079	annotated+fragmen
948	Pirbuterol	1.38	0.000	0.0000	769363	2005024	annotated
971	Suberylglycine	1.94	0.000	0.0000	377691	1453759	annotated
972	Butabarbital	2.34	0.000	0.0000	307734	1561084	annotated
1006	Adenylsuccinic acid	-3.94	0.000	0.0000	803035	52299	annotated+fragmen
1019	PA(20:1(11Z)/0:0)	2.99	0.000	0.0000	193751	1543574	annotated
1032	Aspartyl-Threonine	1.16	0.000	0.0000	719963	1613818	annotated
1071	Nicotinamide D-ribonucleotide	1.82	0.000	0.0000	462518	1635362	annotated+fragmen
1114	riboflavin	2.04	0.000	0.0000	393112	1611531	identified+fragment
1142	Lysyl-Tyrosine	0.12	0.000	0.0000	448209	487388	annotated
1151	(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid	1.15	0.000	0.0000	693752	1544810	annotated
1169	Flavidulol C	2.03	0.000	0.0000	330790	1346425	annotated
1175	L-Coprine	1.38	0.000	0.0000	408875	1061239	annotated
1184	4E,15Z-Bilirubin IXa	2.21	0.000	0.0000	261561	1211029	annotated
1204	1-Methylhypoxanthine	1.77	0.000	0.0000	307127	1050939	annotated
1205	1-Methylinosine	0.89	0.000	0.0000	194811	359904	annotated
1207	7-Aminomethyl-7-carbaguanine	1.11	0.000	0.0000	83347	180235	annotated
1216	5,6-Dihydroxyindole	2.18	0.000	0.0000	190759	861688	annotated
1294	Dihydroferulic acid 4-sulfate	1.52	0.000	0.0000	161047	462874	annotated
1300	Benthiavalicarb isopropyl	0.62	0.000	0.0000	98575	151183	annotated
1316	Methomyl	1.49	0.000	0.0000	365950	1031006	annotated
1353	alpha-linolenic acid	1.58	0.000	0.0000	221371	661736	annotated
1367	L-glycyl-L-hydroxyproline	1.38	0.000	0.0000	411487	1068090	annotated
1453	p-Hydroxyphenylacetothiohydroximate	3.37	0.000	0.0000	72224	749237	annotated
1464	Clobenpropit	1.38	0.000	0.0000	304775	790906	annotated
1472	2-Dimethylamino-5,6-dimethylpyrimidin-4-ol	2.31	0.000	0.0000	170077	842228	annotated

1477	3-Isoxazolidinone	1.97	0.000	0.0000	237766	931417	annotated
1486	Lysyl-Serine	1.89	0.000	0.0000	186745	693443	annotated
1487	N-Methylhistamine	2.41	0.000	0.0000	101214	536953	annotated
1489	Arginyl-Proline	1.73	0.000	0.0000	160596	531138	annotated
1496	PG(18:4(6Z,9Z,12Z,15Z)/0:0)	1.41	0.000	0.0000	59412	158091	annotated
1524	Dehydrocycloxanthohumol hydrate	1.71	0.000	0.0000	135717	443645	annotated
1542	Butalbital	0.74	0.000	0.0000	374082	625273	annotated
1544	Acrylamide	1.18	0.000	0.0000	406408	920530	annotated
1574	Chitobiose	1.38	0.000	0.0000	261420	679299	annotated
1588	O-Desmethylocarvedilol	1.99	0.000	0.0000	39656	157694	annotated
1605	Pentostatin	0.99	0.000	0.0000	240615	476725	annotated
1606	3'-Amino-3'-deoxythymidine	1.33	0.000	0.0000	270345	678453	annotated
1617	FPL64176	2.06	0.000	0.0000	130499	542708	annotated
1656	2-Methylaminoadenosine	1.74	0.000	0.0000	187025	625109	annotated
1699	Ethoxzolamide	2.38	0.000	0.0000	106576	555273	annotated
1746	Galactosylhydroxylysine	1.14	0.000	0.0000	204637	451162	annotated
1786	Tranexamic acid	1.62	0.000	0.0000	154173	473213	annotated
1793	5-Methylcytidine	1.64	0.000	0.0000	145311	452474	annotated
1803	3beta-Hydroxy-5alpha-pregnan-20-one acetate	1.18	0.000	0.0000	214705	484946	annotated
1818	Dimorphecolic acid	1.18	0.000	0.0000	187759	424164	annotated
1855	Isobutyryl-L-carnitine	1.59	0.000	0.0000	96698	291744	annotated
1865	Dihydro-4-mercapto-3(2H)-furanone	0.63	0.000	0.0000	56928	88101	annotated
1874	L-2-Aminoethyl seryl phosphate	1.57	0.000	0.0000	136994	407055	annotated
1878	N-a-Acetyl-L-arginine	1.30	0.000	0.0000	135000	331753	annotated
1930	Oleoylcarnitine	1.31	0.000	0.0000	147893	365529	annotated
1940	Monuron	1.50	0.000	0.0000	110738	313737	annotated
1945	(R)-2-Hydroxysterculic acid	1.55	0.000	0.0000	100755	294545	annotated
2003	Biotin	2.09	0.000	0.0000	8180	34804	annotated

2033	S-Propyl thiosulfate	-2.03	0.000	0.0000	122682	29983	annotated
2036	gamma-Glutamyl-beta-aminopropionitrile	1.10	0.000	0.0000	148565	318375	annotated
2060	Octadecanedioic acid	4.69	0.000	0.0000	11639	299946	annotated
2086	2-Hydroxy-3-methyl-9H-carbazole	-0.81	0.000	0.0000	65520	37342	annotated
2136	Thiophene	1.64	0.000	0.0000	64777	201492	annotated
2137	Penciclovir	1.96	0.000	0.0000	68859	267402	annotated
2232	S-Cystein succinic acid	0.64	0.000	0.0000	54599	85249	annotated
2236	3R-aminononanoic acid	1.59	0.000	0.0000	62485	188495	annotated
2249	2,4-Diamino-6-nitrotoluene	1.64	0.000	0.0000	61773	192989	annotated
2252	Deoxyinosine	2.44	0.000	0.0000	37999	206629	annotated
2256	Acetylcysteine	1.70	0.000	0.0000	32378	105016	annotated
2327	CL(1'-[18:2(9Z,12Z)/0:0],3'-[18:2(9Z,12Z)/0:0])	2.99	0.000	0.0000	23901	190129	annotated
2335	1,4-Diamino-2-nitrobenzene	1.64	0.000	0.0000	57186	177783	annotated
2374	Theasinensin C	1.90	0.000	0.0000	28665	107297	annotated
2419	5-Phosphonoxy-L-lysine	1.55	0.000	0.0000	35864	104723	annotated
2441	xi-4,5-Dihydro-2,4(5)-dimethyl-1H-imidazole	1.37	0.000	0.0000	49912	128925	annotated
2445	N4-Acetylcytidine	1.26	0.000	0.0000	57507	137839	annotated
2465	gamma-Mangostin	1.19	0.000	0.0000	50374	115262	annotated
2744	ethyl tetradecanoate	2.78	0.000	0.0000	83757591	576194752	annotated
2756	PA(18:0/0:0)	-5.59	0.000	0.0000	28021794	580910	annotated
2762	trans-Cinnamate	1.98	0.000	0.0000	133597	526627	annotated
2764	4-Hydroxyphenytoin glucuronide	3.52	0.000	0.0000	24600	282590	annotated
2767	Malate	-1.33	0.000	0.0000	179680172	71351322	annotated+fragmen
2778	D-chiro-Inositol	1.44	0.000	0.0000	56827883	153681054	annotated+fragmen
2779	(1R,2R)-3-[(1,2-Dihydro-2-hydroxy-1-	-4.41	0.000	0.0000	16291504	768147	annotated
2781	2-(2-Thienylmethylene)-1,6-dioxaspiro[4.4]non-3-ene	0.42	0.000	0.0000	286903	385094	annotated
2790	Galactaric acid	0.73	0.000	0.0000	1087431	1806746	annotated
2801	Taurine	1.40	0.000	0.0000	48784079	128870158	identified+fragment

2804	pyrophosphate	-0.20	0.000	0.0000	17188574	14973340	identified
2806	Levogluconan	2.31	0.000	0.0000	1023030	5081199	annotated
2807	3-Ureidopropionate	1.33	0.000	0.0000	1928376	4836027	annotated
2808	3E-methylglutaconic acid	1.30	0.000	0.0000	1174519	2882059	annotated
2809	4,4'-Sulfonyldiphenol	1.42	0.000	0.0000	744983	1995371	annotated
2815	beta-L-Arabinofuranose	0.83	0.000	0.0000	392752	698021	annotated
2820	5-Hydroxy-2-furoic acid	0.92	0.000	0.0000	125230	236706	annotated
2838	CMP	1.79	0.000	0.0000	270903	938746	identified+fragment
2843	D-altro-D-manno-Heptose	2.39	0.000	0.0000	91577	481460	annotated
2845	L-Tyrosine	2.45	0.000	0.0000	91416	501158	annotated
2847	Glucosamine-1P	1.27	0.000	0.0000	190652	459696	annotated
2850	Aspartyl-Glutamine	1.60	0.000	0.0000	93509	283179	annotated
2853	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	1.68	0.000	0.0000	65024	208993	annotated
2856	Pyroglutamylglycine	1.23	0.000	0.0000	49042	114713	annotated
2862	Cinnamyl benzoate	1.86	0.000	0.0000	168641	611564	annotated
2867	sn-Glycerol 3-phosphate	1.34	0.000	0.0000	35165264	88759352	identified+fragment
2872	CMP-N-acetylneuraminat	-6.06	0.000	0.0000	10131947	151468	annotated
2890	2-Oxoglutaramate	0.17	0.000	0.0000	874347	985157	annotated
2903	PC(O-2:0/O-2:0)	1.69	0.000	0.0000	16060	51783	annotated
2904	Pyrrolidonecarboxylic acid	2.30	0.000	0.0000	11163496	55141584	annotated+fragmen
2913	Alloxanthine	2.00	0.000	0.0000	14318570	57367731	annotated+fragmen
2919	Oroselone	-4.14	0.000	0.0000	4009776	228114	annotated
2922	2-Protocatechoylphloroglucinolcarboxylate	1.93	0.000	0.0000	33843	128921	annotated
2923	9-Aminocamptothecin	1.60	0.000	0.0000	38902	117695	annotated
2924	L-alpha-glutamyl-L-hydroxyproline	1.75	0.000	0.0000	18887	63329	annotated
2927	Asparaginyln-Proline	2.72	0.000	0.0000	12332	81344	annotated
2929	Urate	2.02	0.000	0.0000	16197566	65508074	annotated
2930	2,2-Bis(4-hydroxyphenyl)hexafluoropropane	0.94	0.000	0.0000	13137082	25290456	annotated

2937	PI(18:1(9Z)/18:1(11Z))	-2.01	0.000	0.0000	3381128	842084	annotated
2955	Dolichyl phosphate D-mannose	0.74	0.000	0.0000	8499194	14227504	annotated+fragmen
2956	D-Xylulose 5-phosphate	1.76	0.000	0.0000	1141863	3876075	annotated
2957	D-Ribulose 5-phosphate	2.29	0.000	0.0000	790985	3876075	annotated
2959	5-L-Glutamyl-taurine	2.44	0.000	0.0000	534121	2889862	annotated
2962	N-Acetylgalactosamine 6-sulfate	1.47	0.000	0.0000	304713	842093	annotated
2965	7-Hydroxymethyl-12-methylbenz[a]anthracene sulfite	1.73	0.000	0.0000	137212	455853	annotated
2966	D-Glycero-D-galacto-heptitol	4.37	0.000	0.0000	32967	683785	annotated
2973	L-N-Carboxymethylserine	2.00	0.000	0.0000	49363	197096	annotated
2974	D-Galactonate	1.81	0.000	0.0000	11357610	39876192	annotated+fragmen
2990	L-beta-aspartyl-L-glutamic acid	-4.90	0.000	0.0000	3462591	115926	annotated
2993	L-isoleucine	3.10	0.000	0.0000	4029403	34608311	identified
2994	Ovalitenin A	-1.68	0.000	0.0000	1920451	598288	annotated
2998	2'-Deoxysepiapterin	1.33	0.000	0.0000	54103	136384	annotated
3002	Glycyl-Aspartate	-2.54	0.000	0.0000	4302606	740752	annotated
3004	Brugine	1.75	0.000	0.0000	12063	40590	annotated
3005	3-Phospho-DL-glycerate	6.09	0.000	0.0000	390535	26632043	annotated+fragmen
3006	Triphenylsilanol	2.26	0.000	0.0000	586009	2810401	annotated+fragmen
3012	Isosyringinoside	-4.21	0.000	0.0000	1302803	70319	annotated
3014	N-Succinyl-2-L-amino-6-oxoheptanedioate	-3.17	0.000	0.0000	925573	103167	annotated
3032	Norambrinolide	2.67	0.000	0.0000	205333	1305682	annotated
3045	Uracil	2.80	0.000	0.0000	4115962	28617517	annotated
3046	Potassium 2-(1'-ethoxy) ethoxypropanoate	2.66	0.000	0.0000	2018382	12789036	annotated
3047	Homocysteinesulfinic acid	1.90	0.000	0.0000	860002	3199840	annotated
3048	(S)C(S)-S-Methylcysteine sulfoxide	2.09	0.000	0.0000	822948	3514390	annotated
3051	Dihydro-4,6-dimethyl-2-(1-methylethyl)-4H-1,3,5-	0.09	0.000	0.0000	259638	276332	annotated
3054	Astilbin	1.80	0.000	0.0000	17283	60005	annotated
3057	D-Ribonate	1.56	0.000	0.0000	941502	2768111	annotated

3058	1-Isothiocyanato-7-(methylsulfinyl)heptane	0.44	0.000	0.0000	354883	480667	annotated
3062	Urolithin B	0.72	0.000	0.0000	59211	97644	annotated
3066	Orotate	2.17	0.000	0.0000	215523	970790	identified
3069	5'-Dehydroadenosine	1.55	0.000	0.0000	52361	153333	annotated
3083	Fexofenadine	2.06	0.000	0.0000	535774	2228029	annotated
3084	1-Stearoylglycerophosphoinositol	1.15	0.000	0.0000	636911	1417482	annotated+fragmen
3108	Egonol	0.96	0.000	0.0000	64328	125504	annotated
3109	Moracin O	2.00	0.000	0.0000	31427	125504	annotated
3110	Garcimangosone C	4.14	0.000	0.0000	7669	135098	annotated
3115	3-keto-n-caproic acid	3.27	0.000	0.0000	2062480	19849057	annotated
3123	Fosamine	1.81	0.000	0.0000	120897	424467	annotated
3125	Dihydrogen phosphate	1.20	0.000	0.0000	156516	359688	annotated
3127	Tyramine	0.56	0.000	0.0000	65389	96297	annotated
3129	Pseudouridine	1.28	0.000	0.0000	7741759	18832218	annotated+fragmen
3138	L-Aspartyl-L-phenylalanine	-0.69	0.000	0.0000	174364	108258	annotated
3139	Sedoheptulose 1-phosphate	3.07	0.000	0.0000	672843	5635444	annotated+fragmen
3142	Threonic acid	1.67	0.000	0.0000	3067088	9730246	annotated
3153	N-(1-Deoxy-1-fructosyl)threonine	2.81	0.000	0.0000	14181	99495	annotated
3160	6-Hydroxy-2-bornanone glucoside	2.16	0.000	0.0000	13401	59685	annotated
3168	Clidinium	1.82	0.000	0.0000	11789	41647	annotated
3173	(Z,Z)-2-Methyl-5-(8,11,14-pentadecatrienyl)-1,3-	3.13	0.000	0.0000	1304825	11409722	annotated
3175	PG(18:1(9Z)/0:0)	1.01	0.000	0.0000	544658	1096381	annotated
3177	7,9-Tetracosanedione	1.59	0.000	0.0000	138720	416828	annotated
3178	D-Glycerate	2.96	0.000	0.0000	1412379	10962228	annotated+fragmen
3179	Xanthosine	1.76	0.000	0.0000	606473	2058129	annotated+fragmen
3194	Cer(d18:0/16:0)	1.84	0.000	0.0000	326483	1171131	annotated
3196	Cer(d18:1/22:1(13Z))	0.50	0.000	0.0000	121790	171713	annotated
3252	Pyruvic acid	3.06	0.000	0.0000	1065081	8911975	annotated

3256	Salsoline-1-carboxylate	1.19	0.000	0.0000	582091	1325434	annotated
3257	Phenylpropionylglycine	2.74	0.000	0.0000	213630	1428733	annotated
3258	Tetradecanedioic acid	2.78	0.000	0.0000	106352	731240	annotated
3269	6,7-Benzocoumarin	2.40	0.000	0.0000	43328	228919	annotated
3271	a-Methyldopa mono-O-sulfate	1.75	0.000	0.0000	23236	78200	annotated
3276	11-Eicosenoic acid	2.61	0.000	0.0000	1145235	6970220	annotated
3278	5-Hydroxy-7-tetracosanone	0.44	0.000	0.0000	372781	505423	annotated
3280	(S)-3-Hydroxybutanoate	2.18	0.000	0.0000	1421659	6464399	annotated
3293	Glycerophosphoglycerol	1.16	0.000	0.0000	2174752	4874708	annotated
3363	3-(4-Hydroxyphenyl)pyruvate	2.13	0.000	0.0000	1340297	5854959	annotated
3372	Mannitol	3.10	0.000	0.0000	626402	5367772	annotated
3379	Glycyl-Asparagine	-0.17	0.000	0.0000	155361	137962	annotated
3383	desbutyl-lumefantrine	2.14	0.000	0.0000	94891	418121	annotated
3384	Nocardicin F	1.27	0.000	0.0000	81407	196151	annotated
3390	D-4'-Phosphopantothenate	2.09	0.000	0.0000	1325127	5639513	annotated
3402	Kazinol Q	3.19	0.000	0.0000	489167	4472645	annotated
3408	4-Hydroxychalcone	-0.89	0.000	0.0000	191827	103427	annotated
3409	1-Methoxy-2-hydroxyanthracene	1.79	0.000	0.0000	29848	103427	annotated
3414	1-Deoxy-D-altro-heptulose 7-phosphate	2.14	0.000	0.0000	906593	4006951	annotated
3415	ATP	2.09	0.000	0.0000	501366	2129706	annotated+fragmen
3416	5-Oxoavermectin "2a" aglycone	1.70	0.000	0.0000	801072	2606617	annotated+fragmen
3422	L-Tryptophan	1.80	0.000	0.0000	1096132	3826471	identified
3436	sn-Glycero-3-phospho-1-inositol	2.41	0.000	0.0000	683258	3626707	annotated
3482	L-Arabinose	1.58	0.000	0.0000	626375	1877769	annotated
3483	beta-D-Glucosamine	1.11	0.000	0.0000	884015	1909890	annotated
3522	N-Acetyl-alpha-D-galactosamine 1-phosphate	1.99	0.000	0.0000	410362	1632136	annotated
3538	N-lactoyl-Methionine	2.49	0.000	0.0000	506416	2837959	annotated
3543	(all-E)-1,7-bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-one	1.23	0.000	0.0000	72386	169833	annotated

3553	PE(18:1(9Z)/0:0)	1.73	0.000	0.0000	554095	1842874	annotated
3561	D-Biopterin	2.00	0.000	0.0000	31561	126400	annotated
3602	Quinoline yellow	1.63	0.000	0.0000	80184	248386	annotated
3656	1-Pyrroline-5-carboxylic acid	1.74	0.000	0.0000	667383	2223201	annotated
3660	Linoleic acid	2.75	0.000	0.0000	332664	2235004	annotated
3704	Myristicin	1.08	0.000	0.0000	11583	24432	annotated
3713	D-Glucuronic acid	1.32	0.000	0.0000	791164	1980366	annotated+fragmen
3801	2-Oxoglutarate	-1.25	0.000	0.0000	1451488	611201	identified
3811	2-O-Methyl-L-fucose	1.27	0.000	0.0000	304170	732194	annotated
3829	N-Acetyl-alpha-neuraminate	1.28	0.000	0.0000	610083	1485743	annotated
3831	Ethanolamine phosphate	1.21	0.000	0.0000	748986	1738297	identified+fragment
3832	3-O-alpha-D-Glucopyranuronosyl-D-xylose	0.30	0.000	0.0000	362660	447391	annotated
3833	N-Acetyl-L-methionine	3.42	0.000	0.0000	164949	1769274	annotated
3838	4-Aminobutanoate	1.78	0.000	0.0000	432584	1490555	identified
3872	Desmedipham	4.29	0.000	0.0000	11905	232852	annotated
3890	Tetraphyllin B sulfate	2.61	0.000	0.0000	87239	534042	annotated
3891	4-Oxononanal	1.11	0.000	0.0000	636336	1369842	annotated
3892	3-Ethenyl-2,5-dimethyl-4-oxohex-5-en-2-yl acetate	0.68	0.000	0.0000	336331	537413	annotated
3893	(R)-8-Acetoxy-carvotanacetone	1.46	0.000	0.0000	195760	537413	annotated
3908	Methionyl-Methionine	-0.55	0.000	0.0000	87651	60029	annotated
3991	Glycerone phosphate	0.22	0.000	0.0000	425652	494781	annotated
4024	PG(18:2(9Z,12Z)/0:0)	2.87	0.000	0.0000	138390	1008533	annotated
4032	5-Hydroxymethyl-2-furaldehyde	1.27	0.000	0.0000	318103	767503	annotated
4039	3-Sulfinioalanine	2.32	0.000	0.0000	119982	600672	annotated
4044	D-Erythrose 4-phosphate	2.25	0.000	0.0000	129759	617418	annotated
4045	4-[2-(5-Carboxy-2-hydroxy-3-methoxyphenyl)-2-	3.33	0.000	0.0000	35020	351273	annotated
4050	SB 206553	2.44	0.000	0.0000	170356	923784	annotated
4082	Tauropine	2.14	0.000	0.0000	170547	752007	annotated

4142	2-oxo-4-methylthio-butanoic acid	2.71	0.000	0.0000	96572	632625	annotated
4148	1,4-beta-D-Glucan	3.16	0.000	0.0000	14761	131621	annotated
4164	Glycerol 1,2-cyclic phosphate	2.21	0.000	0.0000	144486	666244	annotated
4175	xi-2,2,6-Trimethyl-1,4-cyclohexanedione	0.46	0.000	0.0000	317310	435755	annotated
4194	3-oxo-tetradecanoic acid	2.02	0.000	0.0000	76383	310462	annotated
4220	alpha-Teresantallic acid	1.94	0.000	0.0000	159310	612620	annotated
4253	1-Acetylcyclohexyl acetate	1.38	0.000	0.0000	209607	544081	annotated
4262	Ipomeatetrahydrofuran	-1.38	0.000	0.0000	544519	209592	annotated
4291	PA(18:2(9Z,12Z)/0:0)	0.95	0.000	0.0000	267809	518346	annotated
4292	PE(22:5(7Z,10Z,13Z,16Z,19Z)/14:0)	1.01	0.000	0.0000	263370	529132	annotated
4358	1-Arachidonoylglycerophosphoinositol	2.57	0.000	0.0000	70774	419005	annotated
4367	N-Acetoxy-IQ	1.62	0.000	0.0000	179202	551135	annotated
4379	Indolelactate	2.21	0.000	0.0000	82872	384171	annotated
4388	Danthron	1.60	0.000	0.0000	141777	428459	annotated
4395	UDP	3.07	0.000	0.0000	60363	507453	annotated
4439	Dodecanedioic acid	2.05	0.000	0.0000	74088	305887	annotated
4458	Cyanidin 3-O-(6''-malonyl-arabinoside)	0.62	0.000	0.0000	35018	53857	annotated
4464	Epoxiconazole	-4.84	0.000	0.0000	168504	5900	annotated
4535	5-Hydroxymethyldeoxycytidylate	1.79	0.000	0.0000	89456	309429	annotated
4580	Sulfamoyldapsone	-0.99	0.000	0.0000	332623	167131	annotated
4650	3R-hydroxy-decanoic acid	1.56	0.000	0.0000	103766	306010	annotated
4686	Maltopentaose	2.58	0.000	0.0000	19961	119466	annotated
4726	Hydroxypropyl-Asparagine	1.48	0.000	0.0000	116621	325433	annotated
4739	1-O-Methyl-myo-inositol	1.25	0.000	0.0000	94759	225221	annotated
4742	S-Propyl 2-propene-1-sulfinothioate	1.45	0.000	0.0000	107486	294399	annotated
4743	2-Methylcitric acid	1.31	0.000	0.0000	107425	265557	annotated
4783	Nabam	3.78	0.000	0.0000	20705	283657	annotated
4842	1-(5'-Phosphoribosyl)-5-amino-4-imidazolecarboxamide	1.43	0.000	0.0000	99701	268315	annotated

4848	Valaciclovir	1.27	0.000	0.0000	84980	204594	annotated
4855	D-Glucose 6-sulfate	2.48	0.000	0.0000	32080	178933	annotated
4856	Apigenin 7-sulfate	2.08	0.000	0.0000	44668	189497	annotated
4862	Chondroitin	1.58	0.000	0.0000	57331	171630	annotated
4878	UTP	2.75	0.000	0.0000	22511	151370	annotated
4881	Enalaprilate	2.52	0.000	0.0000	15943	91633	annotated
4889	1-Cyano-2-hydroxy-3-butene	1.74	0.000	0.0000	65752	219817	annotated
4914	Methyl methanesulfonate	1.64	0.000	0.0000	62328	193747	annotated
4954	Sulforaphane-N-acetylcysteine	1.63	0.000	0.0000	52009	161477	annotated
5007	Dihydro-2,4-dimethyl-6-(2-methylpropyl)-4H-1,3,5-	0.79	0.000	0.0000	85846	148904	annotated
5017	Beta-Citryl-L-glutamic acid	1.75	0.000	0.0000	43816	147245	annotated
5180	4-Hydroxymandelate	1.45	0.000	0.0000	54078	147394	annotated
5220	CDP-ribitol	-1.61	0.000	0.0000	103577	33894	annotated
5274	Eriojaposide A	0.44	0.000	0.0000	59283	80288	annotated
5340	lipoamide	0.90	0.000	0.0000	57923	108004	annotated
5350	3,4-Dehydrothiomorpholine-3-carboxylate	2.37	0.000	0.0000	14197	73569	annotated
5436	3-Methoxy-4,5-methylenedioxcinnamaldehyde	2.07	0.000	0.0000	15704	66151	annotated
5490	Hirsutin	1.16	0.000	0.0000	27393	61133	annotated
47	Dichotosinin	-5.75	0.000	0.0001	41997633	781414	annotated
115	trans-4-Hydroxy-L-proline	0.75	0.000	0.0001	99236164	167002196	identified
164	PC(18:1(9Z)/18:1(9Z))	0.94	0.000	0.0001	43350256	83265312	annotated
177	D-2-Aminoheptano-6-lactam	1.16	0.000	0.0001	205569	458771	annotated
275	N,N'-Diacetylhydrazine	0.93	0.000	0.0001	57701	109736	annotated
302	(x)-2-Heptanol glucoside	-4.97	0.000	0.0001	2914063	93222	annotated
309	N-Palmitoylsphingosine	0.96	0.000	0.0001	13977228	27244512	annotated
418	Chrycolide	1.86	0.000	0.0001	29990	108604	annotated
607	Glycidyl oleate	0.44	0.000	0.0001	4989926	6790135	annotated
730	Sphinganine	0.74	0.000	0.0001	2827832	4723892	annotated+fragmen

747	Histidinyl-Threonine	0.73	0.000	0.0001	1174057	1953921	annotated
755	PA(20:4(5Z,8Z,11Z,14Z)e/2:0)	1.17	0.000	0.0001	276309	622057	annotated
788	Histidinyl-Glycine	1.33	0.000	0.0001	1132518	2838395	annotated
794	N-(L-Arginino)succinate	2.52	0.000	0.0001	549979	3159862	annotated+fragmen
878	2,3-Dehydrosalvipisone	-1.36	0.000	0.0001	654977	255865	annotated
917	2-Methoxyestradiol-17beta 3-sulfate	0.96	0.000	0.0001	42174	81838	annotated
1045	Isoputreanine	1.50	0.000	0.0001	567686	1603490	annotated+fragmen
1068	N2-Fructopyranosylarginine	2.83	0.000	0.0001	95524	678992	annotated
1100	Methionyl-Asparagine	0.16	0.000	0.0001	117399	130860	annotated
1165	Histidinyl-Tyrosine	1.01	0.000	0.0001	236783	478343	annotated
1176	Asparaginyln-Histidine	1.24	0.000	0.0001	288705	683909	annotated
1441	PC(P-18:0/16:0)	1.34	0.000	0.0001	417731	1055788	annotated
1485	Glycylprolylhydroxyproline	1.29	0.000	0.0001	384350	938859	annotated
1519	5-Hydroxymethyl-2-furanoate	1.64	0.000	0.0001	300402	934526	annotated
1554	Histidinyl-Asparagine	1.38	0.000	0.0001	263114	683909	annotated
1584	PE(18:3(6Z,9Z,12Z)/0:0)	-0.98	0.000	0.0001	410968	209013	annotated
1631	Captopril	1.37	0.000	0.0001	207679	534975	annotated
1648	Asparaginyln-Valine	0.93	0.000	0.0001	275393	525583	annotated
1649	Glutaminyln-Tyrosine	1.38	0.000	0.0001	143428	373194	annotated
1779	1-Oleoylglycerophosphoserine	1.24	0.000	0.0001	195481	463326	annotated
1795	LysoPE(22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	1.60	0.000	0.0001	156155	474651	annotated
1854	Dieporeticenin	0.88	0.000	0.0001	221204	406259	annotated
1911	Caffeoyl C1-glucuronide	0.85	0.000	0.0001	232000	417804	annotated
1912	2-Methylpyrrole	0.93	0.000	0.0001	177431	338142	annotated
1955	hydroxyisovaleroyl carnitine	1.21	0.000	0.0001	161609	373607	annotated
2144	N-Nitrosodiethylamine	1.35	0.000	0.0001	79790	203521	annotated
2176	apo-[3-methylcrotonoyl-CoA:carbon-dioxide ligase	1.41	0.000	0.0001	79661	211876	annotated
2245	(6RS)-6,19-epidioxy-24,24-difluoro-25-hydroxy-6,19-	1.24	0.000	0.0001	82099	194027	annotated

2258	Isosorbide mononitrate	1.57	0.000	0.0001	67798	200744	annotated
2268	Dihydrozeatin riboside	1.50	0.000	0.0001	48231	136401	annotated
2486	L-Formylkynurenine	0.88	0.000	0.0001	57472	105417	annotated
2597	1-(1-Pyrrolidinyl)-2-propanone	0.59	0.000	0.0001	57387	86387	annotated
2846	Aminofructose 6-phosphate	1.46	0.000	0.0001	167474	459696	annotated
2882	N-Gluconyl ethanolamine phosphate	1.17	0.000	0.0001	1545561	3475695	annotated
2964	Aspartyl-Serine	1.51	0.000	0.0001	240866	685015	annotated
3116	Phenylpyruvate	2.38	0.000	0.0001	1941352	10084624	identified
3284	PI(18:1(9Z)/18:2(9Z,12Z))	1.17	0.000	0.0001	2623531	5883336	annotated
3341	Ethyl hydrogen sulfate	1.83	0.000	0.0001	1557797	5551290	annotated
3342	Ethylphosphate	1.27	0.000	0.0001	730320	1757962	annotated
3719	Ethyl glucuronide	2.12	0.000	0.0001	279871	1215724	annotated
3725	Dambonitol	2.18	0.000	0.0001	88967	402645	annotated
3814	(25R)-1beta,3alpha,7alpha-trihydroxy-5beta-cholestan-	2.11	0.000	0.0001	336950	1458173	annotated
4422	Ethyl 1-(ethylthio)propyl disulfide	1.21	0.000	0.0001	76035	175672	annotated
4925	2,3-Diphenyl-3-(2-pyridinyl)acrylonitrile	1.59	0.000	0.0001	50104	151121	annotated
55	gamma-L-Glutamyl-L-cysteine	0.49	0.000	0.0002	1968682	2772874	annotated+fragmen
244	5-(2-carboxylatoethyl)-4-oxo-4,5-dihydro-1H-imidazol-	2.39	0.000	0.0002	8660059	45482664	annotated
392	L-Theanine	0.78	0.000	0.0002	8102198	13943332	annotated
409	1,4-Dideoxy-1,4-imino-D-ribitol	1.08	0.000	0.0002	3964735	8405593	annotated
454	N-Butyrylglycine	1.05	0.000	0.0002	4245741	8763412	annotated
609	Cohibin C	0.42	0.000	0.0002	3092913	4140183	annotated
711	S-3-oxodecanoyl cysteamine	2.12	0.000	0.0002	840404	3654100	annotated
756	LysoPE(20:3(5Z,8Z,11Z)/0:0)	1.98	0.000	0.0002	135558	533987	annotated
796	Lysyl-Alanine	1.73	0.000	0.0002	1118482	3714930	annotated
798	LysoPC(20:4(8Z,11Z,14Z,17Z))	2.39	0.000	0.0002	392451	2050960	annotated
852	PC(20:3(8Z,11Z,14Z)/20:4(8Z,11Z,14Z,17Z))	1.22	0.000	0.0002	1075265	2504646	annotated
877	Nafenopin	-1.84	0.000	0.0002	915966	255865	annotated

902	Methionyl-Proline	1.19	0.000	0.0002	250287	572619	annotated
1129	N-Despyridinyl rosiglitazone	2.45	0.000	0.0002	280324	1533917	annotated
1156	Lysyl-Leucine	1.46	0.000	0.0002	286012	788285	annotated
1340	Cepharadione B	1.73	0.000	0.0002	308157	1023817	annotated
1556	Domperidone	1.50	0.000	0.0002	305555	865012	annotated
1843	D-myo-Inositol 1,2-cyclic phosphate	1.19	0.000	0.0002	128210	292228	annotated
2126	N-Methylcalystegine C1	1.14	0.000	0.0002	99624	219661	annotated
2127	Linoleamide	1.49	0.000	0.0002	74678	210404	annotated
2505	Normetanephine	1.10	0.000	0.0002	49980	106817	annotated
2830	L-Aspartate	1.38	0.000	0.0002	22753471	59120203	identified
2836	D-Glucono-1,5-lactone	-3.04	0.000	0.0002	8252130	1006279	annotated
2864	(Z)-But-1-ene-1,2,4-tricarboxylate	1.02	0.000	0.0002	123327	249827	annotated
3445	4-[2,2-Dichloro-1-(4-methoxyphenyl)ethenyl]phenol	-3.20	0.000	0.0002	358024	39053	annotated
3484	Methyl 1-(propylsulfinyl)propyl disulfide	-0.47	0.000	0.0002	305545	220832	annotated
4277	Nevirapine	-0.76	0.000	0.0002	448863	265929	annotated
4399	N-Lactoyl ethanolamine phosphate	1.29	0.000	0.0002	178698	435913	annotated
4470	Myricetin 3-arabinoside	1.18	0.000	0.0002	118770	268975	annotated
4522	2-O-beta-D-Glucopyranuronosyl-D-mannose	1.44	0.000	0.0002	78971	214795	annotated
4891	2-Acetyl-3-methylfuran	0.83	0.000	0.0002	119680	213381	annotated
5187	4-N-(N-Acetyl-D-glucosaminy)-protein	1.65	0.000	0.0002	46745	146280	annotated
5423	Quinaprilat	0.77	0.000	0.0002	36903	63062	annotated
135	4-Guanidinobutanoate	0.41	0.000	0.0003	5495350	7278607	annotated+fragmen
308	3-Dehydroxycarnitine	1.36	0.000	0.0003	12874410	32955159	annotated+fragmen
391	PC(20:2(11Z,14Z)/14:1(9Z))	1.36	0.000	0.0003	5862466	15048786	annotated
624	2-Hydroxyadenine	1.14	0.000	0.0003	2301544	5088164	annotated
1516	PC(14:0/0:0)	0.87	0.000	0.0003	367431	670600	annotated
1560	Etorphine	1.21	0.000	0.0003	300763	698118	annotated
1583	L-Cysteine	2.31	0.000	0.0003	56118	278110	annotated

2014	Malonylcarnitine	1.00	0.000	0.0003	121518	243691	annotated
2125	(E,E)-11,13-Octadecadien-9-ynoic acid	1.26	0.000	0.0003	68299	163860	annotated
3015	Methyl benzoate	-1.49	0.000	0.0003	506072	180445	annotated
3144	(1R,2S)-1-Hydroxypropane-1,2,3-tricarboxylate	1.37	0.000	0.0003	957059	2469955	annotated
3145	Isocitrate	1.41	0.000	0.0003	931879	2469955	annotated
3446	4,4'-Thiodianiline	1.51	0.000	0.0003	13406	38120	annotated
3460	citrate	1.81	0.000	0.0003	519062	1816243	identified
3555	Demeton-O	1.38	0.000	0.0003	518581	1351503	annotated
4057	UDP-D-Xylose	1.92	0.000	0.0003	118074	448255	annotated+fragmen
4106	4-Deoxyerythronic acid	1.40	0.000	0.0003	259185	682577	annotated
4241	cis-Aconitate	1.09	0.000	0.0003	86911	185059	identified
4913	Sulfoglycolithocholate(2-)	-1.34	0.000	0.0003	132546	52241	annotated
5395	(Z)-[3-(Methylsulfinyl)-1-propenyl] 2-propenyl disulfide	1.13	0.000	0.0003	36885	80805	annotated
218	Hydroxyprolyl-Arginine	1.68	0.000	0.0004	125865	403065	annotated
220	Glycyl-Glutamine	1.08	0.000	0.0004	191222	403294	annotated
287	PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	1.17	0.000	0.0004	114508	257875	annotated
511	PE(24:1(15Z)/16:1(9Z))	0.58	0.000	0.0004	224714	336613	annotated
1474	2-Pyrroloylglycine	2.33	0.000	0.0004	201804	1013403	annotated
1538	FAD	0.67	0.000	0.0004	505134	805405	identified+fragment
2584	Dihydro-3(2H)-thiophenone	0.80	0.000	0.0004	45686	79720	annotated
2709	Hyperforin	-0.88	0.000	0.0004	29569	16067	annotated
2936	Tauro-b-muricholic acid	1.42	0.000	0.0004	17208493	45987860	annotated+fragmen
3117	3-Methyldioxyindole	-2.90	0.000	0.0004	550788	73593	annotated
3143	(1S,2S)-1-Hydroxypropane-1,2,3-tricarboxylate	0.46	0.000	0.0004	1794357	2469955	annotated
3264	Withaperuvine H	-3.70	0.000	0.0004	1327213	101978	annotated
3994	PS(22:0/0:0)	1.34	0.000	0.0004	128605	324800	annotated
4084	Ethyl 2-hydroxyisovalerate	0.99	0.000	0.0004	213508	424618	annotated
4209	Thiosulfuric acid	2.18	0.000	0.0004	121464	548560	annotated

4806	Sphingosine 1-phosphate	1.23	0.000	0.0004	103808	244126	annotated
4898	2',3'-Cyclic UMP	1.76	0.000	0.0004	40963	138939	annotated
4911	Vulgarole	0.70	0.000	0.0004	105822	171494	annotated
113	PE-NMe(18:1(9Z)/18:1(9Z))	0.66	0.000	0.0005	114450582	181016032	annotated
675	S-Propyl-L-cysteine	1.16	0.000	0.0005	1033826	2308002	annotated+fragmen
681	PE(20:0/14:1(9Z))	0.54	0.000	0.0005	3606239	5225583	annotated
927	7-oxo-8-amino-nonanoic acid	0.40	0.000	0.0005	486799	642511	annotated
1647	N-Stearoylsphingosine	1.10	0.000	0.0005	288236	617152	annotated
2270	Prunetin	1.19	0.000	0.0005	76843	175669	annotated
3894	Methyl benzoate	-0.73	0.000	0.0005	1083908	654252	annotated
4282	Oxalosuccinate	-0.60	0.000	0.0005	312255	206605	annotated
5468	Norfluoxetine	0.50	0.000	0.0005	47745	67712	annotated
5480	6-(Hydroxymethyl)-2,4(1H,3H)-pteridinedione	1.24	0.000	0.0005	28414	66950	annotated
46	Adenosine	-1.04	0.000	0.0006	135073003	65544613	identified+fragment
185	PC(20:3(5Z,8Z,11Z)/16:1(9Z))	0.91	0.000	0.0006	37108046	69875003	annotated
680	Sphingosine	1.18	0.000	0.0006	2782604	6325993	annotated+fragmen
904	Gamma-glutamyl-Methionine	1.17	0.000	0.0006	95551	214294	annotated
989	Threoninyl-Glutamine	1.12	0.000	0.0006	357346	776833	annotated
1067	delta-Guanidinovaleric acid	1.50	0.000	0.0006	255303	719732	annotated
1713	Protoanemonin	1.20	0.000	0.0006	173398	399303	annotated
2434	Glucosylisomaltol	0.79	0.000	0.0006	58386	101080	annotated
3274	IMP	1.56	0.000	0.0006	2058766	6052992	annotated+fragmen
3387	Indolepyruvate	1.80	0.000	0.0006	1471646	5115874	annotated
3958	(-)-1-Methylpropyl 1-propenyl disulfide	1.28	0.000	0.0006	317305	772738	annotated+fragmen
4683	Terpendole K	2.26	0.000	0.0006	7694	36782	annotated
4792	gamma-L-Glutamyl-gamma-L-glutamyl-L-methionine	2.54	0.000	0.0006	20198	117280	annotated
4901	6,8-Di-O-methylaverufin	0.92	0.000	0.0006	38909	73542	annotated
5295	(Z)-6-Tetradecene-1,3-diyne-5,8-diol	-0.12	0.000	0.0006	48181	44259	annotated

114	PE(22:2(13Z,16Z)/15:0)	0.53	0.000	0.0007	125511358	181016032	annotated
222	L-2-Amino-3-(1-pyrazolyl)propanoic acid	3.01	0.000	0.0007	7166034	57602985	annotated
442	Isogingerenone B	-0.71	0.000	0.0007	9608314	5869051	annotated
836	PE(20:2(11Z,14Z)/14:0)	1.06	0.000	0.0007	1622462	3371414	annotated
1359	1-(2H-1,3-Benzodioxol-5-yl)-2-[2,6-dimethoxy-4-(prop-	0.89	0.000	0.0007	51712	95845	annotated
1456	Kiwiionoside	1.53	0.000	0.0007	313222	901435	annotated
2073	Clitidine	1.71	0.000	0.0007	72526	237221	annotated
3244	6-bromo-eicosa-5E,9Z-dienoic acid	2.44	0.000	0.0007	9620	52357	annotated
3519	Hexadecanedioic acid	-3.55	0.000	0.0007	1045016	88963	annotated
4556	Butylmethacrylate (+ isobutylmethacrylate)	0.68	0.000	0.0007	256888	410446	annotated
988	Gamma-glutamyl-Threonine	0.52	0.000	0.0008	544113	781327	annotated
1905	1-Pyrroline	0.39	0.000	0.0008	232230	303877	annotated
3039	Xanthosine 5'-phosphate	1.06	0.000	0.0008	864577	1806098	annotated
3236	Prorepensin	1.22	0.000	0.0008	55902	130051	annotated
4513	Azelaic acid	1.05	0.000	0.0008	183511	379167	annotated
629	Histidinyl-Lysine	-2.09	0.000	0.0009	777718	183033	annotated
1549	Glycyl-Serine	0.68	0.000	0.0009	327636	526692	annotated
1998	N-Acetyl-L-tyrosine	0.18	0.000	0.0009	68472	77331	annotated
2201	Temurin	1.57	0.000	0.0009	56997	169342	annotated
2947	Trimetaphosphoric acid	-1.22	0.000	0.0009	580946	250021	annotated
4288	6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one	0.38	0.000	0.0009	450452	585250	annotated
5325	Thiophanate-methyl	1.14	0.000	0.0009	48620	106980	annotated
51	Homocarnosine	1.26	0.000	0.0010	1778013	4254862	annotated+fragmen
2120	3-Keto-scylo-inosamine	0.82	0.000	0.0010	102040	179618	annotated
2473	8-Oxodeoxycoformycin	0.40	0.000	0.0010	65477	86662	annotated
2605	Threoninyl-Tryptophan	1.02	0.000	0.0010	37630	76393	annotated
4072	Valeric acid	0.52	0.000	0.0010	512388	735214	annotated
4703	3alpha,7alpha,16alpha,24R-Tetrahydroxy-5beta-	1.63	0.000	0.0010	86776	268529	annotated

4993	Procymidone	0.41	0.000	0.0010	48923	64931	annotated
672	Lysyl-Valine	1.55	0.000	0.0011	1403496	4098320	annotated
1050	2,6-Dibromohydroquinone	-1.14	0.000	0.0011	285221	129133	annotated
1073	PC(2:0/0:0)	1.20	0.000	0.0011	469420	1074790	annotated
1085	Phytosphingosine	0.57	0.000	0.0011	939202	1390622	annotated
1504	Methylimidazole acetaldehyde	-0.59	0.000	0.0011	840124	557128	annotated
1518	Allocystathionine	1.23	0.000	0.0011	153198	358422	annotated+fragmen
1645	2-Amino-4-hydroxy-6-pteridinecarboxylic acid	2.48	0.000	0.0011	109521	609629	annotated
2094	N-Acetyldehydroanoinine	0.58	0.000	0.0011	175296	262027	annotated
2373	6-Keto-decanoylcarnitine	0.74	0.000	0.0011	60384	100586	annotated
2446	1-Methylseleno-N-acetyl-D-galactosamine	1.92	0.000	0.0011	19004	71728	annotated
3394	Brosimone I	-2.13	0.000	0.0011	337475	77252	annotated
4085	Lumichrome	1.04	0.000	0.0011	142532	294080	annotated
49	Tolbutamide	-3.02	0.000	0.0012	476924	58764	annotated
1527	Gamma-glutamyl-Valine	1.03	0.000	0.0012	316829	648491	annotated
1599	Benzenepropanenitrile	-1.30	0.000	0.0012	703295	285653	annotated
2138	Microlenin	1.08	0.000	0.0012	106275	224739	annotated
2938	Sulfate	2.64	0.000	0.0012	1979641	12374594	annotated
3099	2-oxoglutarate(2-)	-1.57	0.000	0.0012	1971107	665902	annotated
4680	Asparaginy-Gamma-glutamate	0.44	0.000	0.0012	42716	58004	annotated
685	N(pi)-Methyl-L-histidine	1.50	0.000	0.0013	1951399	5531401	identified+fragment
1766	S-Phenylmercapturic acid	2.31	0.000	0.0013	96110	477964	annotated
2310	PG(P-18:0/18:4(6Z,9Z,12Z,15Z))	1.70	0.000	0.0013	55200	178761	annotated
4392	Mandelonitrile sophoroside	1.06	0.000	0.0013	241807	505735	annotated
1433	PS(18:0/0:0)	0.76	0.000	0.0014	491448	830302	annotated
4895	(+)-5-Deoxykievitone	0.65	0.000	0.0014	117997	185030	annotated
314	Isoleucyl-Alanine	1.57	0.000	0.0015	5661963	16863045	annotated
364	PC(20:3(8Z,11Z,14Z)/18:2(9Z,12Z))	0.80	0.000	0.0015	9275433	16135078	annotated

1028	5-Methylthio-D-ribose	0.99	0.000	0.0015	859017	1703688	annotated
1099	Histidiny-Valine	0.64	0.000	0.0015	683935	1066579	annotated
4218	Phenindione	1.28	0.000	0.0015	110468	268420	annotated
1864	Homocysteine	0.73	0.000	0.0016	115433	191597	annotated
1970	4-Pyridoxate	0.64	0.000	0.0016	133805	207870	annotated
3028	N6-Carbamoyl-L-threonyl-adenosine	-2.51	0.000	0.0016	113792	19957	annotated
3222	trans-Aconitate	0.60	0.000	0.0016	462054	700945	annotated
3820	Seriny-Threonine	1.09	0.000	0.0016	622487	1324082	annotated
3476	Monoethyl malonic acid	1.34	0.000	0.0017	1198615	3025848	annotated+fragmen
4036	Glycyl-Threonine	1.14	0.000	0.0017	422951	934681	annotated
4389	Monomethyl sulfate	1.05	0.000	0.0017	177073	367872	annotated
2263	N-Acetylputrescine	1.02	0.000	0.0018	88370	179749	annotated+fragmen
5385	5,6-Dihydrouridine	0.81	0.000	0.0018	50120	87934	annotated
605	PS(18:0/20:4(8Z,11Z,14Z,17Z))	-0.44	0.000	0.0019	6733977	4968862	annotated
957	PS(18:0/16:0)	0.79	0.000	0.0020	1251759	2161448	annotated
1391	Methionyl-Leucine	1.28	0.000	0.0020	441078	1073026	annotated
2302	2-Phenylacetamide	0.54	0.000	0.0020	129455	187824	annotated
2579	3',5'-Cyclic AMP	0.80	0.000	0.0020	47721	83125	identified
252	PC(18:0/0:0)	0.99	0.000	0.0021	13189268	26177930	annotated+fragmen
4169	cis-alpha-octenoic acid	0.79	0.000	0.0021	403581	700231	annotated
428	PE(20:0/15:0)	0.77	0.000	0.0022	8405316	14295899	annotated
854	(R)C(R)S-S-Propylcysteine sulfoxide	0.09	0.000	0.0022	339989	362388	annotated
3455	Lauric acid	0.98	0.000	0.0022	1796323	3550735	annotated
630	Histidiny-Arginine	2.00	0.000	0.0023	32700	130377	annotated
1950	Diisopropyl sulfate	0.86	0.000	0.0023	107987	196078	annotated
2388	N-(1-Deoxy-1-fructosyl)tyrosine	1.77	0.001	0.0023	18019	61404	annotated
4174	Ethyl tiglate	0.64	0.000	0.0023	430678	669283	annotated
5134	Avenic acid A	0.81	0.001	0.0023	79246	138796	annotated

2616	Acetoxyacetone	0.63	0.001	0.0024	34319	53122	annotated
1602	PE(24:1(15Z)/14:1(9Z))	0.75	0.001	0.0026	440140	741115	annotated
2589	Valclavam	2.14	0.001	0.0026	16770	74004	annotated
3081	Sulfinpyrazone	-4.71	0.001	0.0026	1567370	59737	annotated
1780	L-Cystine	2.00	0.001	0.0027	70546	282266	identified
5455	Picolinoylglycine	1.09	0.001	0.0027	29796	63393	annotated
455	Leucyl-Valine	1.45	0.001	0.0028	4057695	11051608	annotated
2571	20:3-Glc-Campesterol	0.37	0.001	0.0029	12416	16019	annotated
3209	2-Hydroxy-2-(2-oxopropyl)butanedioic acid	0.10	0.001	0.0029	6296612	6767633	annotated
3478	Imidazoleacetic acid ribotide	1.50	0.001	0.0029	1120301	3174944	annotated
4880	Eugenitin	1.83	0.001	0.0029	52296	185311	annotated
9	Creatine	0.42	0.001	0.0030	681424712	913604224	annotated+fragmen
441	L-Homocitrulline	2.08	0.001	0.0030	2167565	9162851	annotated
828	Acetone cyanohydrin	0.71	0.001	0.0030	1763040	2880018	annotated
1122	Sodium sulfate	0.88	0.001	0.0030	668886	1234760	annotated
1313	Hypotaurocyamine	1.53	0.001	0.0030	178651	517641	annotated
2798	Clonidine	0.90	0.001	0.0030	72426	134875	annotated
4605	5'-Oxoinosine	0.44	0.001	0.0031	206962	280796	annotated
1403	p-Hydroxyfelbamate	1.53	0.001	0.0033	232046	672003	annotated
285	LysoPC(20:3(5Z,8Z,11Z))	-0.11	0.001	0.0034	417401	385546	annotated
879	N-Jasmonoyltyrosine	-2.14	0.001	0.0034	555701	126042	annotated
925	Styrene	-0.76	0.001	0.0034	2272411	1342424	annotated
1018	Tyrosyl-Valine	-0.15	0.001	0.0034	143127	129145	annotated
760	PE(20:1(11Z)/15:0)	1.92	0.001	0.0035	689647	2611611	annotated
1394	Glycyl-Arginine	2.23	0.001	0.0035	203207	951654	annotated
1307	11-amino-undecanoic acid	-0.60	0.001	0.0036	445926	293884	annotated
1526	N,N-Dimethylhistidine	1.46	0.001	0.0036	273807	754689	annotated
1610	1-Methoxyppyrene	2.10	0.001	0.0037	149819	642867	annotated

1155	Isoleucyl-Arginine	0.86	0.001	0.0038	452227	821877	annotated
1392	Esprocarb	0.29	0.001	0.0038	215755	263161	annotated
4258	2-Phosphinomethylmalate	1.16	0.001	0.0038	249846	558749	annotated
4554	a-L-threo-4-Hex-4-enopyranuronosyl-D-galacturonic	-0.32	0.001	0.0038	88410	70593	annotated
1164	Glycyl-Tyrosine	0.68	0.001	0.0040	705713	1129363	annotated
2451	N-lactoyl-Tryptophan	0.34	0.001	0.0040	47644	60138	annotated
905	Alanyl-Tryptophan	0.99	0.001	0.0041	71815	142258	annotated
2400	Mephenytoin	0.96	0.001	0.0041	68780	134094	annotated
3029	Hydramethylnon	-4.01	0.001	0.0042	54294	3370	annotated
3883	Benzoyl glucuronide (Benzoic acid)	-1.15	0.001	0.0042	442105	199186	annotated
843	PC(20:3(8Z,11Z,14Z)/20:2(11Z,14Z))	0.98	0.001	0.0043	1674713	3297964	annotated
2108	Dinex	0.56	0.001	0.0043	95957	141730	annotated
458	Vorinostat	1.24	0.002	0.0044	709318	1675341	annotated
4033	D-Glucosamine	0.23	0.002	0.0044	107671	126161	identified
5475	Fukiic acid	1.26	0.002	0.0045	18102	43253	annotated
3885	UDP-glucuronate	-1.58	0.002	0.0046	439445	147021	annotated+fragmen
1734	alpha-Sinensal	-1.42	0.002	0.0047	484791	181531	annotated
4812	S-Allyl-L-cysteine	0.93	0.002	0.0047	91693	175262	annotated
242	N-Methylnicotinate	0.97	0.002	0.0048	14257470	27910652	annotated+fragmen
5313	Dorzolamide	1.31	0.002	0.0048	34632	85578	annotated
906	Dihydroclavaminic acid	1.02	0.002	0.0049	69360	140318	annotated
2638	4-O-alpha-D-Galactopyranosylcalystegine B2	0.87	0.002	0.0049	35917	65867	annotated
1497	Mitiglinide	1.70	0.002	0.0050	48977	159553	annotated
3132	Ezetimibe	-1.74	0.002	0.0050	2993895	896955	annotated
2413	Methionyl-Aspartate	1.18	0.002	0.0051	48315	109377	annotated
1157	Histidiny-Glutamine	0.95	0.002	0.0052	298211	576138	annotated
4378	D-Arabinitol 1-phosphate	0.79	0.002	0.0052	142447	245606	annotated
5101	Epoxyanethole	0.42	0.002	0.0054	73057	97910	annotated

3696	(-)-Quebrachitol	1.46	0.002	0.0055	434194	1191274	annotated
1873	Dihydrobiopterin	0.37	0.002	0.0056	232164	299516	annotated
1988	15beta-Hydroxy-7alpha-mercapto-pregn-4-ene-3,20-	-0.41	0.002	0.0056	141217	106245	annotated
4265	CDP-ethanolamine	0.73	0.002	0.0057	336816	557163	annotated
1189	Histidinal	1.30	0.002	0.0058	387210	956631	annotated
5462	Ascorbic acid-2-sulfate	1.27	0.002	0.0058	26119	63100	annotated
2535	N-Nitrosodi-n-butylamine	1.55	0.002	0.0061	16251	47747	annotated
3065	(x)-1,2-Propanediol 1-O-b-D-glucopyranoside	2.17	0.002	0.0061	94975	428000	annotated
5193	Sedoheptulose 1,7-bisphosphate	0.66	0.002	0.0061	44324	69850	annotated
4782	1-Isothiocyanato-7-(methylthio)heptane	0.67	0.002	0.0062	117135	186066	annotated
2897	DOPA sulfate	1.71	0.003	0.0064	60545	198425	annotated
179	PE(22:1(13Z)/15:0)	0.95	0.003	0.0065	37434553	72201018	annotated
611	PG(18:1(9Z)/18:1(11Z))	-0.12	0.003	0.0066	1196925	1099045	annotated
898	Isoleucyl-Serine	1.31	0.003	0.0066	784190	1949379	annotated
256	Amino adipic acid	1.52	0.003	0.0067	13766150	39516097	annotated
262	cis-3-Hexenyl b-primeveroside	-6.10	0.003	0.0067	4352662	63315	annotated
1867	6-Acetylpicropolin	0.75	0.003	0.0067	239716	403244	annotated
1436	Gamma-glutamyl-Gamma-glutamate	0.52	0.003	0.0068	246805	352702	annotated
1437	N2-Succinoylarginine	0.78	0.003	0.0068	205850	352702	annotated
2601	Synephrine acetone	0.60	0.003	0.0069	40275	61123	annotated
608	PS(18:0/18:0)	0.53	0.003	0.0070	4081302	5884721	annotated
958	1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione	1.02	0.003	0.0071	705984	1427915	annotated
496	SM(d18:1/16:0)	-0.16	0.003	0.0072	8311218	7426577	annotated
1035	PE(22:5(7Z,10Z,13Z,16Z,19Z)/16:0)	0.87	0.003	0.0075	1133859	2076765	annotated
715	Valeryl glycine	0.69	0.003	0.0076	1338782	2159637	annotated
2797	1-(Isothiocyanatomethyl)-4-methoxybenzene	-1.30	0.003	0.0076	313922	127876	annotated
772	PE(20:0/16:1(9Z))	1.25	0.003	0.0078	1386029	3300959	annotated
1191	Alpha-CEHC	-1.30	0.003	0.0079	829268	336398	annotated

3509	Phenylacetic acid	-0.63	0.003	0.0080	2500431	1617797	annotated
2518	2,5-Dihydro-2,4,5-trimethylthiazole	0.79	0.003	0.0081	38802	67295	annotated
343	Brunfelsamidine	1.65	0.004	0.0085	5468322	17117155	annotated
1162	N-Acetylphenylalanine beta-naphthyl ester	-1.00	0.004	0.0085	600468	299708	annotated
144	2-O-(6-Phospho-alpha-mannosyl)-D-glycerate	1.22	0.004	0.0086	1176233	2734056	annotated+fragmen
3839	Uridine diphosphate glucose	1.55	0.004	0.0088	248744	727604	annotated+fragmen
2025	Isonicotinic acid	0.36	0.004	0.0089	150945	193348	annotated
4924	SC-58125	1.54	0.004	0.0089	39618	115469	annotated
88	L-Carnitine	0.98	0.004	0.0090	76387582	151080370	identified+fragment
2197	Hydroxypropyl-Glutamine	0.89	0.004	0.0090	62681	115925	annotated
2273	N-Acetylvanilalanine	1.27	0.004	0.0090	70624	169861	annotated
2497	Aspartyl-Arginine	0.59	0.004	0.0095	70505	106108	annotated
5153	Ethyl 10-undecenoate	0.80	0.004	0.0096	66098	115052	annotated
438	(3S)-3-Hydroxy-L-enduracididine	0.32	0.004	0.0097	2298186	2874948	annotated
959	CDP-choline	0.59	0.004	0.0097	1469776	2214194	annotated+fragmen
5243	1D-myo-Inositol 1,4-bisphosphate	1.15	0.004	0.0097	33581	74538	annotated
5363	(3xi,6xi)-Cyclo(alanylvalyl)	0.57	0.005	0.0102	52911	78780	annotated
2288	Methionyl-Threonine	0.71	0.005	0.0103	75064	123021	annotated
2070	Threoninyl-Tyrosine	0.86	0.005	0.0104	127676	230953	annotated
899	Histidinyl-Leucine	0.06	0.005	0.0106	607466	631297	annotated
4180	PA(P-20:0/22:4(7Z,10Z,13Z,16Z))	-0.25	0.005	0.0106	515961	434574	annotated
4516	9-Octadecenoic acid 1-[[[(1-oxohexadecyl)oxy]methyl]-	0.51	0.005	0.0110	167667	238489	annotated
4171	Polypropylene glycol (m w 1,200-3,000)	0.13	0.005	0.0112	186741	204132	annotated
4043	Pyrocatechol sulfate	1.37	0.005	0.0117	123929	321278	annotated
1756	(R)-3-hydroxybutyrylcarnitine	0.70	0.005	0.0118	179720	292848	annotated
5410	3-hydroxy-undecanoic acid	0.63	0.006	0.0120	47271	73243	annotated
433	S-(Hydroxyphenylacetothiohydroximoyl)-L-cysteine	0.35	0.006	0.0122	3763780	4799938	annotated
3828	4-Methoxybenzyl formate	1.36	0.006	0.0127	308987	793997	annotated

683	PA(18:0/20:4(5Z,8Z,11Z,14Z))	-2.27	0.006	0.0130	816498	168926	annotated
4649	Stearoylglycerone phosphate	1.24	0.006	0.0130	73354	173755	annotated
2358	N1-Methyl-2-pyridone-5-carboxamide	0.69	0.006	0.0131	58008	93433	annotated
3344	3-Deoxy-D-manno-octulosonate 8-phosphate	-0.43	0.006	0.0134	112091	83090	annotated
1065	(2R,3R)-3-Methylglutamyl-5-semialdehyde-N6-lysine	0.90	0.006	0.0135	203615	380701	annotated
352	5-Guanidino-3-methyl-2-oxopentanoate	2.34	0.006	0.0136	2113983	10701153	annotated
4236	L-phenylalanyl-L-hydroxyproline	0.83	0.006	0.0136	135641	241500	annotated
3948	trans-Grandmarin	0.25	0.007	0.0141	21560	25698	annotated
838	S-Allylcysteine	0.59	0.007	0.0147	1567241	2359568	annotated
1692	3-Hydroxystigmast-5-en-7-one	0.90	0.007	0.0149	118256	221406	annotated
4693	Kinobscurinone	1.37	0.007	0.0149	60183	155507	annotated
3962	Hydroxycotinine	-0.30	0.007	0.0153	532005	430956	annotated
4064	S-Nitrosoglutathione	0.98	0.008	0.0154	166806	329506	annotated
5128	4,5-Dihydrovomifoliol	0.66	0.008	0.0154	92539	146712	annotated
3359	UMP	0.87	0.008	0.0161	3038461	5543097	identified+fragment
186	PC(20:3(8Z,11Z,14Z)/20:3(8Z,11Z,14Z))	-0.54	0.008	0.0163	14242149	9802820	annotated
810	Ethyl N-methylantranilate	0.82	0.008	0.0166	517448	911990	annotated+fragmen
1690	(2R,2'S)-Isobuteine	1.04	0.008	0.0167	223570	459887	annotated
4530	3-oxo capric acid	0.87	0.008	0.0170	168521	307975	annotated
3096	Methylphosphate	1.52	0.009	0.0172	5137975	14745461	annotated
1132	Methionine sulfoxide	0.63	0.009	0.0174	692536	1074735	annotated
346	Ophthalmic acid	0.90	0.009	0.0185	9931282	18541271	annotated+fragmen
5170	1-(Malonylamino)cyclopropanecarboxylic acid	1.66	0.009	0.0186	31123	98526	annotated
2370	PS(16:0/22:1(11Z))	0.64	0.009	0.0188	95838	149438	annotated
192	Leu-Gly-Pro	-4.14	0.010	0.0192	5133821	291875	annotated
4009	4-Hydroxycyclohexylcarboxylic acid	0.45	0.010	0.0198	639344	871302	annotated
1838	TetraHCA	0.97	0.010	0.0199	218198	426757	annotated
1848	PE(14:0/18:0)	0.84	0.010	0.0202	168411	301231	annotated

3486	Phenylpropanoate	1.46	0.011	0.0207	253116	696951	annotated
1451	2-O-Methylcytosine	0.78	0.011	0.0212	304135	522592	annotated
3487	3-Succinoylpyridine	-0.63	0.011	0.0212	134954	87398	annotated
4131	thymine	0.53	0.011	0.0212	487737	704716	identified+fragment
1916	O-glutaroyl-L-carnitine	0.68	0.011	0.0214	140188	223961	annotated
811	2(N)-Methyl-norsalsolinol	0.83	0.011	0.0215	512385	911990	annotated+fragmen
1536	Pseudoecgonine	0.90	0.011	0.0215	386406	723011	annotated
2218	(R,S)-Nicotine	-0.51	0.011	0.0215	165147	116125	annotated
4701	Glycyl-Tryptophan	0.41	0.011	0.0216	30674	40889	annotated
5358	2E,6E-Octadienal	0.99	0.011	0.0216	36204	71908	annotated
1654	Fluenetil	1.12	0.012	0.0224	255248	553805	annotated
1327	PE-Cer(d14:1(4E)/22:0(2OH))	-0.05	0.012	0.0225	180812	174936	annotated
2618	S-Sulfanylglutathione	0.95	0.012	0.0225	21956	42416	annotated
625	Guanosine	0.60	0.012	0.0233	2014382	3053325	identified+fragment
122	Glutathione	0.73	0.012	0.0234	58357330	96906724	annotated+fragmen
111	4-(beta-Acetylaminoethyl)imidazole	1.35	0.012	0.0237	41624876	106293944	identified+fragment
617	Fenugreekine	-0.60	0.012	0.0237	3641521	2408344	annotated+fragmen
797	Arginyl-Threonine	0.15	0.012	0.0237	709012	785788	annotated
3850	Metsulfovax	0.23	0.013	0.0238	1267905	1488366	annotated
1995	PE(20:3(5Z,8Z,11Z)/15:0)	0.51	0.013	0.0240	247102	351301	annotated
5586	Chlorendic acid	-0.94	0.013	0.0241	23733	12373	annotated
628	Alanyl-Arginine	1.75	0.013	0.0246	1682176	5674355	annotated
2606	Homoveratric acid	0.92	0.013	0.0247	30593	57942	annotated
1365	PC(O-16:0/18:2(9Z,12Z))	0.79	0.014	0.0255	572149	989268	annotated
4823	Ferulate	0.50	0.014	0.0263	59368	84203	annotated
1030	PE(20:0/18:3(6Z,9Z,12Z))	1.15	0.014	0.0264	793628	1758113	annotated
2866	Phenol	1.49	0.014	0.0269	1573929	4427977	annotated
4172	3-Hydroxy-2-methyl-[S-(R,R)]-butanoic acid	0.94	0.016	0.0289	228821	440168	annotated

1491	Gamma-glutamyl-Phenylalanine	0.61	0.016	0.0291	222222	339292	annotated
5	Glycerophosphocholine	0.46	0.016	0.0300	123065808	168762646	annotated
3148	Propane-1,2-diol 1-phosphate	-0.71	0.016	0.0302	292603	178411	annotated
2132	Phenylacetonitrile	0.53	0.017	0.0308	168944	243621	annotated
2396	Kanzonol V	0.17	0.017	0.0308	132787	149577	annotated
2182	Artemoin A	0.56	0.017	0.0311	133552	196827	annotated
1907	Flavoxate	0.83	0.017	0.0312	211157	375340	annotated
1133	L-Albizziine	1.25	0.018	0.0320	512653	1220861	annotated
10	Streptidine	-7.15	0.018	0.0334	101561357	714286	annotated
38	L-Glutamine	1.06	0.018	0.0334	127467776	266107672	identified+fragment
1490	Glycyl-Phenylalanine	0.89	0.018	0.0334	380395	706188	annotated
5047	Asparaginy-Serine	0.60	0.019	0.0338	79315	120607	annotated
5141	PG(21:0/17:2(9Z,12Z))	0.32	0.019	0.0338	60658	75940	annotated
2525	Primidolol	1.08	0.019	0.0345	42427	89497	annotated
1532	PC(P-18:0/0:0)	0.90	0.021	0.0369	311917	580814	annotated
3712	(R)-2,3-Dihydroxypropane-1-sulfonate	1.01	0.021	0.0375	682839	1379777	annotated
832	Trimethylamine N-oxide	0.70	0.021	0.0376	1222010	1981130	annotated
1014	Isoleucyl-Threonine	0.54	0.021	0.0380	519645	756341	annotated
1760	Diethanolamine	0.76	0.022	0.0385	195693	331485	annotated
1852	N,2,3-Trimethyl-2-(1-methylethyl)butanamide	-0.39	0.022	0.0389	257957	196906	annotated
1796	1-Palmitoylglycerophosphoinositol	0.68	0.022	0.0399	160886	258126	annotated
1044	N-Formyl-4-amino-5-aminomethyl-2-methylpyrimidine	0.32	0.023	0.0412	935817	1167928	annotated
856	PE(20:3(5Z,8Z,11Z)/16:1(9Z))	0.61	0.023	0.0413	1878708	2875516	annotated
1435	Gamma-glutamyl-Serine	0.37	0.024	0.0416	485893	625891	annotated
1928	NeuAalpha2-3Galbeta-Cer(d18:1/16:0)	0.23	0.025	0.0432	283198	331743	annotated
674	DL-2-amino-octanoic acid	1.00	0.025	0.0433	2679979	5360429	annotated
1870	N-Methylcalystegine B2	0.45	0.025	0.0436	298379	408694	annotated
1910	PC(P-18:1(11Z)/18:0)	0.59	0.025	0.0443	242871	365442	annotated

841	Glycopeptide	0.93	0.026	0.0447	748583	1427588	annotated
2116	S-Allyl-L-cysteine	1.04	0.026	0.0450	57858	119290	annotated
1627	3-keto palmitic acid	0.12	0.026	0.0453	135534	147715	annotated
3793	S-(4-Bromophenyl)-mercaptopyruvate	-0.86	0.026	0.0458	95325	52351	annotated
872	7-Methylguanine	0.70	0.026	0.0459	1460867	2366784	annotated
1593	Xanthopterin-B2	0.95	0.027	0.0460	28634	55332	annotated
4182	Sulfolithocholyglycine	0.64	0.027	0.0463	479374	746797	annotated
4026	N-Acetyl-L-aspartate	0.93	0.027	0.0468	403902	770856	annotated
974	PC(O-20:0/12:0)	0.69	0.027	0.0472	1342393	2164825	annotated
294	Ectoine	0.71	0.028	0.0476	13639407	22358918	annotated+fragmen
310	Cer(d18:1/24:1(15Z))	-0.99	0.028	0.0476	4013986	2021917	annotated
900	Hydroxypropyl-Lysine	0.66	0.028	0.0483	414930	655406	annotated
2215	Isocarbamid	0.79	0.028	0.0484	74027	127628	annotated
2588	xi-2,5-Dihydro-2,4-dimethylthiazole	0.60	0.029	0.0491	41100	62213	annotated

CTL T24h vs CTS T24h

<i>Peak id</i>	<i>Metabolite</i>	<i>Log FC</i>	<i>P-value</i>	<i>Adjusted P-value</i>	<i>Peak intensity CTL T24h</i>	<i>Peak intensity CTS T24h</i>	<i>Identification</i>
460	Cysteinyl-Tyrosine	//	0.0000	0.0000	0	52136	annotated
461	Hexahomomethionine	//	0.0000	0.0000	0	31056	annotated
471	5,6-Dihydroxyprostaglandin F1a	//	0.0000	0.0000	70279	0	annotated
1627	3-keto palmitic acid	//	0.0000	0.0000	40942	0	annotated
1937	S-Acetylphosphopantetheine	//	0.0000	0.0000	28163	0	annotated
2060	Octadecanedioic acid	-0.59	0.0000	0.0000	133344	88445	annotated
2764	4-Hydroxyphenytoin glucuronide	//	0.0000	0.0000	70909	0	annotated
4039	3-Sulfinioalanine	//	0.0000	0.0000	27995	0	annotated
4188	Saccharin	//	0.0000	0.0000	0	293576	annotated
4783	Nabam	//	0.0000	0.0000	0	23186	annotated
4934	Acetyl-CoA	//	0.0000	0.0000	18583	0	annotated
479	Demethylphosphinothricin	//	0.0000	0.0001	12171	0	annotated
2040	Triethylene Glycol Monomethyl Ether	-1.69	0.0000	0.0004	190496	59041	annotated
355	D-Glucosyldihydrosphingosine	3.14	0.0000	0.0007	1054181	9300889	annotated
1311	2,3-Butanediol glucoside	2.84	0.0000	0.0010	95706	687176	annotated
3114	Licoricone	//	0.0000	0.0025	3763	0	annotated
4171	Polypropylene glycol (m w 1,200-3,000)	2.22	0.0001	0.0048	116456	544030	annotated
3979	Fucose 1-phosphate	2.19	0.0004	0.0268	84886	386563	annotated
2966	D-Glycero-D-galacto-heptitol	-1.82	0.0005	0.0380	176531	49878	annotated
2003	Biotin	//	0.0007	0.0470	5348	0	annotated

CTL T48h vs CTS T48h

<i>Peak id</i>	<i>Metabolite</i>	<i>Log FC</i>	<i>P-value</i>	<i>Adjusted P-value</i>	<i>Peak intensity CTL T48h</i>	<i>Peak intensity CTS T48h</i>	<i>Identification</i>
47	5,6-Dihydroxyprostaglandin F1a	//	0.0000	0.0000	0	70169	annotated
499	Difloxacin	//	0.0000	0.0000	0	59371	annotated
2060	Octadecanedioic acid	//	0.0000	0.0000	0	33464	annotated
3114	Licoricone	//	0.0000	0.0000	0	5704	annotated
3811	2-O-Methyl-L-fucose	//	0.0000	0.0000	0	149324	annotated
3890	Tetraphyllin B sulfate	//	0.0000	0.0000	0	93940	annotated
4050	SB 206553	//	0.0000	0.0000	36022	0	annotated
4913	Sulfoglycolithocholate(2-)	//	0.0000	0.0000	33868	0	annotated
4934	Acetyl-CoA	-3.37	0.0000	0.0000	119626	11592	annotated
5350	3,4-Dehydrothiomorpholine-3-carboxylate	//	0.0000	0.0000	0	8610	annotated
3004	Brugine	//	0.0000	0.0001	4965	0	annotated
4364	Coenzyme A	-2.66	0.0000	0.0009	381352	60202	annotated
479	Demethylphosphinothricin	//	0.0000	0.0010	0	7142	annotated
4148	1,4-beta-D-Glucan	1.42	0.0001	0.0089	25553	68222	annotated
3390	D-4'-Phosphopantothenate	1.07	0.0004	0.0374	1515119	3188843	annotated